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Use of Models in Managing Ground-Water Protection Programs

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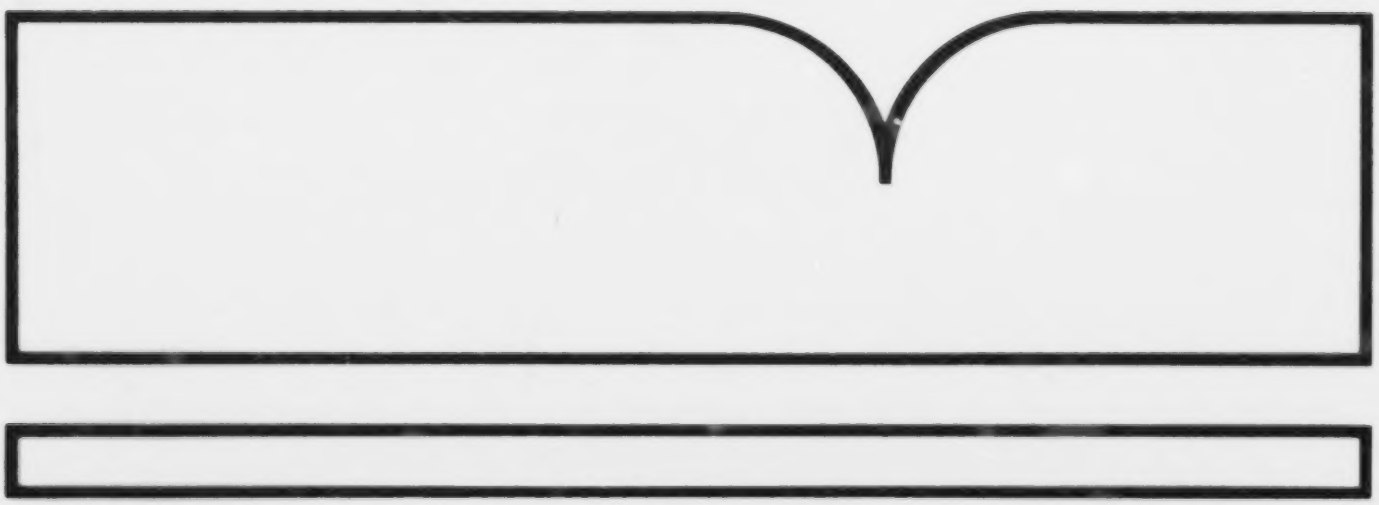

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THE USE OF MODELS IN MANAGING GROUND-WATER PROTECTION PROGRAMS

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FOREWORD

The U.S. Environmental Protection Agency was established to coordinate administration of the major Federal programs designed to protect the quality of our environment.

An important part of the Agency's effort involves the search for information about environmental problems, management techniques and new technologies through which optimum use of the Nation's land and water resources can be assured and the threat pollution poses to the welfare of the American people can be minimized.

EPA's Office of Research and Development conducts this search through a nationwide network of research facilities.

As one of the facilities, the Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, the unsaturated zone and the saturated zones of the suburface environment; (b) define the processes to be used in characterizing the soil and subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil and indigenous organisms; and (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

This report contributes to that knowledge which is essential in order for EPA to establish and enforce pollution control standards which are reasonable, cost effective and provide adequate environmental protection for the American public.

Clinton W. Hall
Director
Robert S. Kerr Environmental
Research Laboratory

ABSTRACT

Because ground-water quality protection is emerging as a major National environmental problem of this decade, there is increasing pressure on regulators and the regulated to identify, assess or even anticipate situations involving ground-water contamination. Site-specific and generic mathematical models are increasingly being used by EPA to fulfill its mandates under a number of major environmental statutes which call for permit issuance, investigation of potential problems, remediation activities, exposure assessment and a myriad of other policy decisions.

Mathematical models can be helpful tools to managers of ground-water protection programs. They may be used for testing hypotheses about conceptualizations and to gather a fuller understanding of important physical, chemical and biological processes which affect ground-water resources. The possible outcomes of complex problems can be addressed in great detail, if adequate data are available. The success of these efforts depends on the accuracy and efficiency with which the natural processes controlling the behavior of ground water, and the chemical and biological species it transports, are simulated. Success also depends heavily on the expertise of the modeler and the communication with management so that the appropriateness, underlying assumptions, and limitations of specific models are appreciated.

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CHAPTER 1
THE UTILITY OF MODELS

INTRODUCTION

Every time man attempts to simulate the effects of natural phenomena, he is engaging in the scientific art of modeling. Models are nothing more than simplified representations of reality, and their creation and use involves a considerable degree of subjective judgment, as well as an attempt to incorporate known scientific facts. There are many forms of models, each having specific advantages and disadvantages compared with the remainder.

Physical models, such as sand-tanks used to simulate aquifers (Figure 1-1) and laboratory columns used to study the relative motion of various contaminants flowing through aquifer materials (Figure 1-2), provide an element of reality which is enlightening and satisfying from an intuitive viewpoint. Their main disadvantage relates to the extreme efforts and time required to generate a meaningful amount of data. Other difficulties relate to the care required to obtain samples of subsurface material for construction of these models, without significantly disturbing the natural condition of the samples.

Analog models are also physically based, but their operating principle is one of similarity, not true-life representation. A typical example is the electric analog model (Figure 1-3), in which capacitors and resistors are able to closely replicate the effects of the rate of release of water from storage in aquifers. The clear disadvantage is that 'a camel is not a horse', even if both can carry a load. As is the case with other physically based models, data generation is slow and there is little flexibility for experimental design changes.

Mathematical models are non-physical, relying instead on the quantification of relationships between specific parameters and variables to simulate the effects of natural processes (Figure 1-4). As such, mathematical models are abstract and provide little in the way of a directly observable link to reality. Despite this lack of intuitive grace, mathematical models can generate powerful insights into the functional dependencies between causes and effects in the real world. Large amounts of data can be generated quickly, and experimental modifications can be made with minimal effort, so

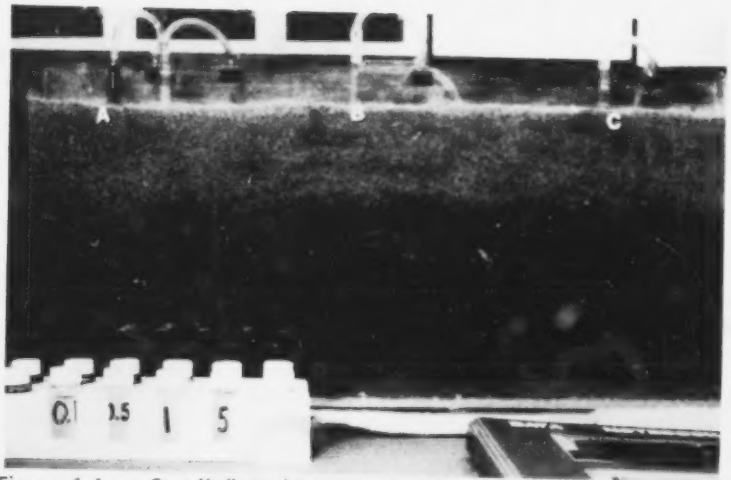

Figure 1-1. Small "sand tank" physical aquifer model. Three Pumping wells (A,B,C) penetrate the homogeneous sand to study the effects of well hydraulics on plume movements. Vials in foreground contain various concentrations of water-active dyes.

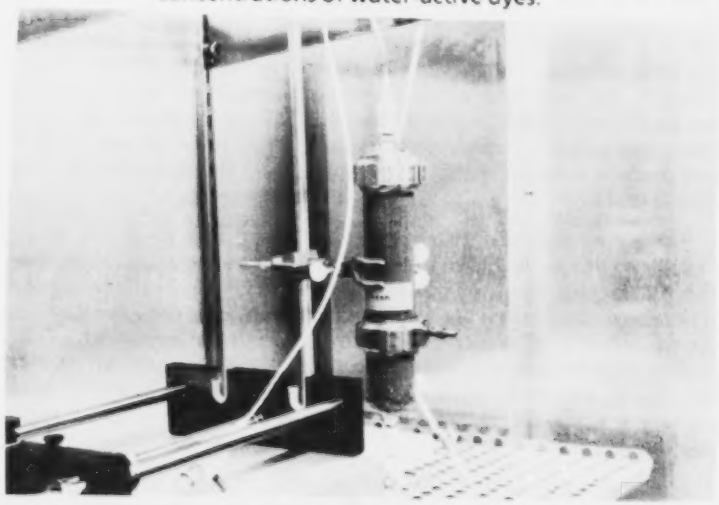

Figure 1-2. Laboratory column housed in constant-temperature environmental chamber. Contaminated solutions are injected into column through inlet tubing in top, by action of hydraulic press in foreground. Samples of the advancing front are withdrawn through ports visible on right-hand side and bottom of column.

Figure 1-3. Electric analog aquifer model constructed by Illinois State Water Survey. The regular array of resistors and the two electric "pumps" shown are hard-wired into a board covered with the appropriate geologic maps.

that many possible situations can be studied in great detail for a given problem.

MANAGEMENT APPLICATIONS

Mathematical models can and have been used to help organize the essential details of complex ground-water management problems so that reliable solutions are obtained (Holcomb Research Institute, 1976; Bachmat and others, 1978; U.S. Office of Technology Assessment, 1982; van der Heijde and others, 1985). Some principal areas where mathematical models are now being used to assist in the management of ground-water protection are:

(1) appraising the physical extent, and chemical and biological quality, of ground-water reservoirs (e.g., for planning purposes),
(2) assessing the potential impact of domestic, agricultural, and industrial practices (e.g., for permit issuance),
(3) evaluating the probable outcome of remedial actions at waste sites, and aquifer restoration techniques generally, and
(4) providing health-effects exposure estimates.

The success of these efforts depends on the accuracy and efficiency with which the natural processes controlling the behavior of ground water, and the chemical and biological species it transports, are simulated (Boonstra and de Ridder, 1976; Mercer

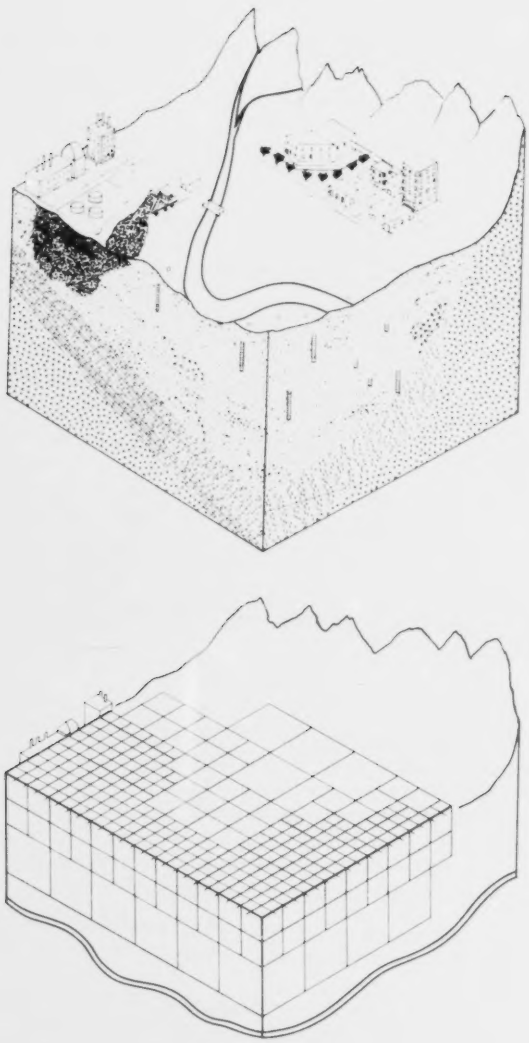

Figure 1-4. Typical ground-water contamination scenario and a possible contaminant transport model grid design for its simulation. Values for natural process parameters would be specified at each node of the grid in performing simulations. The grid density is greatest at the source and at potential impact locations.

and Faust, 1981; Wang and Anderson, 1982). The accuracy and efficiency of the simulations, in turn, are heavily dependent on subjective judgements made by the modeler and management.

In the current philosophy of ground-water protection programs, the value of a ground-water resource is bounded by the most beneficial present and future uses to which it can be put (U.S. EPA, 1984). In most instances, physical appraisals of ground-water resources are conducted within a framework of technical and economic classification schemes. Classification of entire ground-water basins by potential yield is a typical first step (Domenico, 1972). After initial identification and evaluation of a ground-water resource, strategies for its rational development need to be devised.

Development considerations include the need to protect vulnerable recharge areas and the possibility of conjunctive use with available surface waters (Kazmann, 1972). Ground-water rights must be fairly administered to assure adequate supplies for domestic, agricultural, and industrial purposes. Because basinwide or regional resource evaluations normally do not provide sufficent resolution for water allocation purposes, more detailed characterizations of the properties and behavior of an aquifer, or of a subdivision of an aquifer, are usually needed. Hence, subsequent classifications may involve local estimation of net annual recharge, rates of outflow, and the pumpage which can be substained without undesirable effects.

The consequences of developments which might affect ground-water quality may be estimated initially by employing generalized classification schemes; for example, classifications based on regional hydrogeologic settings have been presented (Heath, 1982; Aller and others, 1985). Very detailed databases, however, must be created and molded into useful formats before decisions can be made on how best to protect and rehabilitate ground-water resources from site-specific incidents of natural and manmade contamination.

The latter are ordinary ground-water management functions which benefit from the use of mathematical models. There are other uses, however, which ought to be considered by management. The director of the International Ground Water Modeling Center discussed the role of modeling in the development of ground-water protection policies recently, noting its success in many policy formulation efforts in the Netherlands, the United States, and Israel. Nevertheless, he concluded that modeling was not widely relied upon for decision-making by managers; the primary obstacle has been an inability of modelers and program managers to communicate effectively (van der Heijde, 1985). The top executives of a leading high-tech ground-water contamination consulting firm made the same point clearly, going on to highlight the need for qualified personnel appreciative of the appropriateness, underlying assumptions, and limitations of specific models (Faust and others,

1981). Because these views are widely held by technical professionals, it will be emphasized herein that mathematical models are useful only within the context of the assumptions and simplifications on which they are based. If managers are mindful of these factors, however, mathematical models can be a tremendous asset in the decision- making process.

MODELING CONTAMINANT TRANSPORT

Associated with most hazardous waste sites is a complex array of chemical wastes and the potential for ground-water contamination. The hydrogeologic settings of these sites are usually quite complicated when examined at the scale appropriate for technical assessments and remediation efforts (e.g., 100's of feet). As a result, data acquisition and interpretation methods are needed that can examine to an unprecendented degree the physical, chemical, and biological processes that control the transport and fate of ground-water contaminants. The methods and tools that have been in use for large-scale characterizations (e.g., regional water quality studies) are applicable in concept to the specialized needs of hazardous waste site investigations; however, the transition to local-scale studies is not without scientific and economic consequences. In part, this stems from the highly variable nature of contaminant distributions at hazardous waste sites; but it also results from the limitations of the methods, tools, and theories used. Proper acknowledgement of the inherent limitations means that one must project the consequences of their use within the framework of the study at hand.

Assessments of the potential for contaminant transport require interdisciplinary analyses and interpretations. Integration of geologic, hydrologic, chemical, and biological approaches into an effective contaminant transport evaluation can only be possible if the data and concepts invoked are sound. The data must be accurate, precise, and appropriate at the intended problem scale. Just because a given parameter (e.g., hydraulic conductivity) has been measured correctly at certain points with great reproducibility, is no guarantee that those estimates represent the volumes of aquifer material assigned to them by a modeler. The degree to which the data are representative, therefore, is not only relative to the physical scale of the problem, it is relative to the conceptual model to be used for interpretation efforts. It is crucial, then, to carefully define and qualify the conceptual model. In so doing, special attention should be given to the possible spatial and temporal variations of the data that will be collected.

To circumvent the impossibly large numbers of measurements and samples which would be needed to eliminate all uncertainties regarding the true relationships of parameters (e.g., hydraulic conductivity) and variables (e.g., contaminant concentrations and rates of movement), more comprehensive theories are constantly

under development. The use of newly developed theories to help solve field problems, however, is often a frustrating exercise. Most theoretical advances call for some data which are not yet practically obtainable (e.g., chemical interaction coefficients, relative permeabilities of immiscible solvents and water, etc.). The 'state-of-the-art' in contaminant transport assessments is necessarily a compromise between the sophistication of 'state-of-the-science' theories, the current limitations regarding the acquisition of specific data, and economics. In addition, the best attempts to obtain credible data are limited by natural and anthropogenic variabilities; and these lead to the need for considerable judgement on the part of the professional.

Despite these technical limitations, how well the problem is conceptualized remains the most serious concern in modeling efforts. For example, researchers recently produced dramatic evidence to show that, in spite of detailed field measurements, extrapolations of two-dimensional model results to a truly three-dimensional problem lead to wildly inaccurate projections of the actual behavior of the system under study (Molz and others, 1983). Therefore, it is incumbent on model users to recognize the difference between an approximation and a misapplication. Models should never be used strictly on the basis of familiarity or convenience; an appropriate model should always be sought.

CATEGORIES OF MODELS

The foregoing is not meant to imply that appropriate models exist for all ground-water problems, because a number of natural processes have yet to be fully understood. This is especially true for ground-water contaminant transport evaluations, where the chemical and biological processes are still poorly defined. For, although great advances have been made concerning the behavior of individual contaminants, studies of the interactions between contaminants are still in their infancy. Even the current understanding of physical processes lags behind what is needed, such as in the mechanics of multiphase flow and flow through fractured rock aquifers. Moreover, certain well-understood phenomena pose unresolved difficulties for mathematical formulations, such as the effects of partially penetrating wells in unconfined (water-table) aquifers.

The technical-use categories of models are varied, but they can be grouped as follows (Bachmat and others, 1978; van der Heijde and others, 1985):

(1) parameter identification models,
(2) prediction models,
(3) resource management models, and
(4) data manipulation codes.

Parameter identification models are most often used to estimate the aquifer coefficients determining fluid flow and contaminant transport characteristics, like annual recharge (Puri, 1984), coefficients of permeability and storage (Shelton, 1982; Khan, 1986a and b), and dispersivity (Guven and others, 1984; Strecker and Chu, 1986). Prediction models are the most numerous kind of model, and abound because they are the primary tools for testing hypotheses about the problem one wishes to solve (Andersen and others, 1984; Mercer and Faust, 1981; Krabbenhoft and Anderson, 1986).

Resource management models are combinations of predictive models, constraining functions (e.g., total pumpage allowed) and optimization routines for objective functions (e.g., optimization of wellfield operations for minimum cost or minimum drawdown/pumping lift). Very few of these are so well developed and fully supported that they may be considered practically useful, and there does not appear to be a significant drive to improve the situation (van der Heijde, 1984a and 1984b; van der Heijde and others, 1985). Data manipulation codes also have received little attention until recently. They are now becoming increasingly popular, because they simplify data entry ('preprocessors') to other kinds of models and facilitate the production of graphic displays ('postprocessors') of the data outputs of other models (van der Heijde and Srinivasan, 1983; Srinivasan, 1984; Moses and Herman, 1986). Other software packages are available for routine and advanced statistics, specialized graphics, and database management needs (Brown, 1986).

CHAPTER SUMMARY

Mathematical models can be helpful tools to managers of ground-water protection programs. They may be used for testing hypotheses about conceptualizations and to gather a fuller understanding of important physical, chemical, and biological processes which affect ground-water resources. The possible outcomes of complex problems can be addressed in great detail, if adequate data are available. Mathematical modeling is neither simple nor impossible, but its successful application relies heavily on the expertise of the modeler and the degree of communication with management.

The merits of any problem solving technique need to be judged by many criteria, the most important of which may not relate to mathematical sophistication. Qualitative judgements by prior experience, 'back of the envelope' calculations, analytical models, and other non-numerical modeling methods should be considered for a reason which deserves emphasis; the data available or obtainable may not justify extensive numerical model analyses (Javendel and others, 1984). After all, it is neither pretty nor efficient to 'use a silver sledgehammer to drive a thumbtack'.

CHAPTER 2
ASSUMPTIONS, LIMITATIONS, AND QUALITY CONTROL

INTRODUCTION

There are many natural processes that affect chemical transport from point to point in the subsurface. These natural processes can be arbitrarily divided into three categories: physical, chemical, and biological (Table 2-1). Conceptually, contaminant transport in the subsurface is an undivided phenomenon composed of these processes and their interactions (Figure 2-1). At this level the transport process may be gestalt: the sum of its parts, measured separately, may not equal the whole because of interactions between the parts. In the theoretical context, a collection of scientific laws and empirically derived relationships comprise the overall transport process. The universally shared premise that underlies theoretical expressions is that there are no interactions, measureable or otherwise.

Significant errors may result from the discrepancy between conceptual and theoretical appproaches. Also the simplifications of theoretical expressions used to solve practical problems can cause substantial errors in the most careful analyses. Assumptions and simplifications, however, must often be made in order to obtain mathematically tractable solutions. Because of this, the magnitude of errors that arise from each assumption and simplification must be carefully evaluated. The phrase, "magnitude of errors", is emphasized because highly accurate evaluations usually are not possible. Even rough approximations are rarely trivial exercises because they frequently demand estimates of some things which are as yet ill-defined.

PHYSICAL PROCESSES

Until recently, ground-water scientists studied physical processes to a greater degree than chemical or biological processes. This bias resulted in large measure from the fact that, in the past, ground-water practitioners dealt mostly with questions of adequate water supplies. As quality considerations began to dominate ground-water issues, the need for studies of the chemical and biological factors, as well as more detailed representations of the physical factors, became apparent.

Table 2-1. **Natural processes that affect subsurface contaminant transport.**

PHYSICAL PROCESSES
Advection (porous media velocity)
Hydrodynamic Dispersion
Molecular Diffusion
Density Stratification
Immiscible Phase Flow
Fractured Media Flow
CHEMICAL PROCESSES
Oxidation-Reduction Reactions
Radionuclide Decay
Ion-Exchange
Complexation
Co-Solvation
Immiscible Phase Partitioning
Sorption
BIOLOGICAL PROCESSES
Microbial Population Dynamics
Substrate Utilization
Biotransformation
Adaptation
Co-metabolism

There are two complimentary ways to view the physical processes involved in subsurface contaminant transport: the piezometric (pressure) viewpoint and the hydrodynamic viewpoint. Ground-water problems of yesterday could be addressed by the former, such as solving for the change in pressure head caused by pumping wells. Contamination problems of today also require detailed analyses of wellfield operations, for example, pump-and-treat plume removals. However, solutions to such problems depend principally on hydrodynamic evaluations, such as computing ground-water velocity (advection) distributions and dispersion estimates for migrating plumes.

Advection and Dispersion

Ground-water velocity distributions can be approximated if the variations in hydraulic conductivity, porosity, and the strength and location of recharge and discharge sources can be estimated.

While there are several field and laboratory methods for estimating hydraulic conductivity, these are not directly comparable because different volumes of aquifer material are

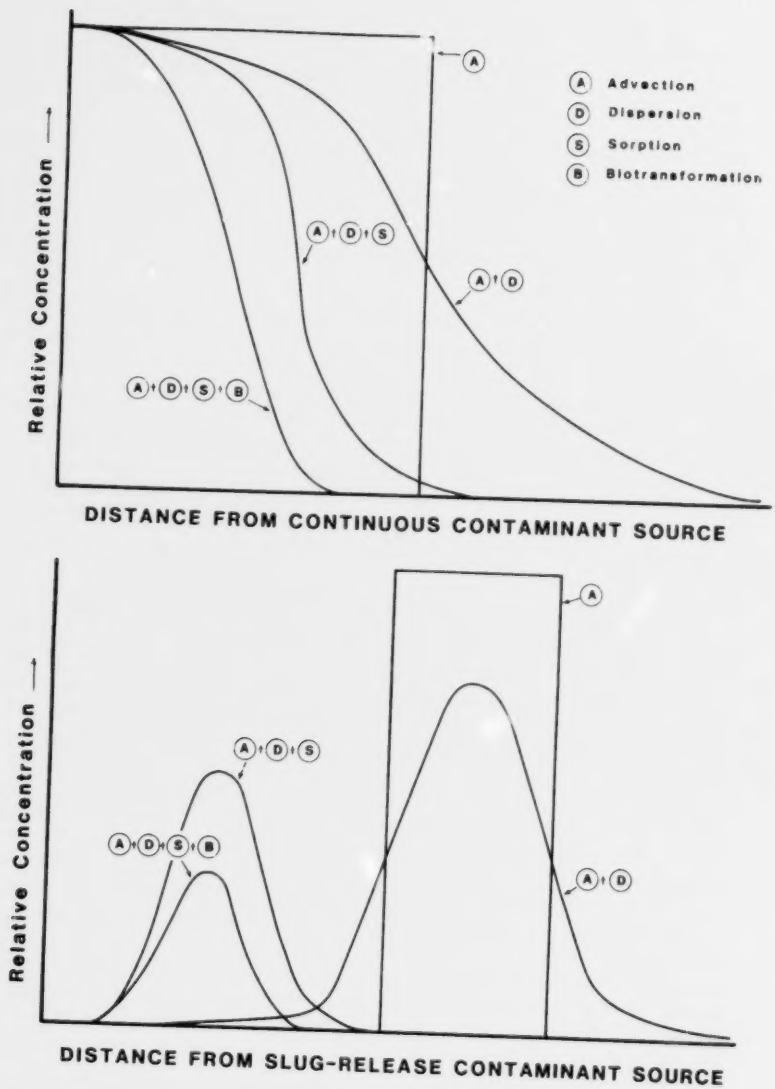

Figure 2-1. The Influence of natural processes on levels of contaminants downgradient from continuous and slug-release sources.

affected by different tests. Laboratory permeameter tests, for example, obtain measurements from small core samples and thus give point value estimates. These tests are generally reliable for consolidated rock samples, such as sandstone, but can be highly unreliable for unconsolidated samples, such as sands, gravels, and clays. Pumping tests give estimates of hydraulic conductivity that are averages over the entire volume of aquifer subject to the pressure changes induced by pumping. These give repeatable results, but they are often difficult to interpret. Tracer tests are also used to estimate hydraulic conductivity in the field, but are difficult to conduct properly.

Regardless of the estimation technique used, the best that can be expected is order-of-magnitude estimates for hydraulic conductivity at the field scale appropriate for site-specific work. Conversely, porosity estimates that are accurate to better than a factor of two can be obtained. Estimation of the strength of nonpoint sources of recharge to an aquifer, such as infiltrating rainfall and leakage from other aquifers, is another order-of-magnitude effort. Similarly, nonpoint sources of discharge, such as aquifer losses to gaining streams, are difficult to quantify. Estimation of the strength of point sources of recharge or discharge (injection or pumping wells) can be highly accurate.

Consequently, it is not possible to generalize the quality of velocity distributions. They may be accurate to within a factor of two for very simple aquifers, but are more often accurate to an order-of-magnitude only. This situation has changed little over the past 20 years because better field and laboratory methods for characterizing velocity distributions have not been developed. This, however, is not the primary difficulty associated with defining the advective part of contaminant transport in the subsurface. The primary difficulty is that field tests for characterizing the physical parameters that control velocity distributions are not incorporated into contamination investigations on a routine basis. The causes seem to be: a perception that mathematical models can 'back-out' an approximation of the velocity distribution (presumably eliminating the need for field tests); unfamiliarity with field tests by many practitioners; and a perception that field tests are too expensive. A more field oriented approach is preferable because the non-uniqueness of modeling results has been amply demonstrated, and this leads to uncertain decisions regarding the design of remedies.

Dispersion estimates are predicated on velocity distribution estimates and their accuracy is therefore directly dependent on the accuracy of the estimated hydraulic conductivity distribution. Tracer tests have been the primary method used to determine dispersion coefficients until recently. Presently there are suggestions that any field method capable of generating a detailed understanding of the spatial variability of hydraulic conductivity, which in turn could give an accurate representation of the velocity

distribution, may be used to derive estimates of dispersion coefficients. The manner in which data from field tests should be used to derive estimates of dispersion coefficients, however, is a controversial issue. There are both deterministic and stochastic schools of thought, and neither has been conclusively demonstrated in complex hydrogeological settings.

Complicating Factors

Certain subtleties of the spatial variability of hydraulic conductivity must be understood because of its key role in the determination of velocity distributions and dispersion coefficients. Hydraulic conductivity is also known as the coefficent of permeability because it is comprised of fluid factors as well as the intrinsic permeability of the stratum in question. This means that a stratum of uniform intrinsic permeability (which depends strictly on the arrangement of its pores) may have a wide range of hydraulic conductivity because of differences in the density and viscosity of fluids that are present. The result is a dramatic downward shift in local flow directions near plumes that have as little as a 1% increase in density relative to uncontaminated water. Such density contrasts frequently occur at landfills and waste impoundments. It is often necessary to correct misimpressions of the direction of a plume because density considerations were not addressed.

Many solvents and oils are highly insoluble in water, and may be released to the subsurface in amounts sufficient to form a separate fluid phase. Because that fluid phase will probably have viscosity and density different from freshwater, it will flow at a rate and, possibly, in a direction different from that of the freshwater with which it is in contact. If an immiscible phase has density approximately the same or less than that of ground water, this phase will not move down past the capillary fringe of the ground water. Instead, it will flow along the top of the capillary fringe in the direction of the maximum water-level elevation drop. If the density of an immiscible phase is substantially greater than the ground water, the immiscible phase will push its way into the ground water as a relatively coherent blob. The primary direction of its flow will then be down the dip of the first impermeable stratum encountered. There is a great need for better means of characterizing such behavior for site-specific applications. Currently, estimation methods are patterned after multiphase oil reservoir simulators. One of the key extensions needed is the ability to predict the transfer of trace levels of contaminants from the immiscible fluid to ground water, such as xylenes from gasoline.

Anisotropy is a subtlety of hydraulic conductivity which relates to structural trends of the rock or sediments of which an aquifer is composed. Permeability and hydraulic conductivity are directionally dependent in anisotropic strata. When molten material from deep underground crystallizes to form granitic or

basaltic rocks, for instance, it forms cleavage planes which may later become the preferred directions of permeability. Marine sediments accumulate to form sandstone, limestone, and shale sequences that have much less vertical than horizontal permeability. The seasonal differences in sediments that accumulate on lakebeds, and the stratification of grain sizes deposited by streams as they mature, give rise to similar vertical-to-horizontal anisotropy. Streams also cause anisotropy within the horizontal plane, by forming and reworking their sediments along a principal axis of movement. These structural variations in permeability would be of minimal concern except that ground water does not flow at right angles to water-level elevation contours under anisotropic conditions. Instead, flow proceeds along oblique angles, with the degree of deviation from a right-angle pathway proportional to the amount of anisotropy. This fact is all too often ignored and the causes again seem to be a reluctance to conduct the proper field tests, combined with an over-reliance on mathematical modeling.

If the pathways created by cleavage planes and fractures begin to dominate fluid flow through a subsurface stratum, the directions and rates of flow are no longer predictable by the equations used for porous rock and sediments. There have been a number of attempts to represent fractured flow as an equivalent porous medium, but these tend to give poor predictions when major fractures are present and when there are too few fractures to guarantee a minimum degree of interconnectedness. Other representations that have been studied are various dual porosity models, in which the bulk matrix of the rock has one porosity and the fracture system has another. Further development of the dual porosity approach is limited by the difficulty in determining a transfer function to relate the two different porosity schemes. Research in this area needs to be accelerated because there is a great likelihood of fractured flow in just those situations commonly believed to be the most suitable for disposal of hazardous wastes, such as building landfills on 'impermeable' bedrock.

Considerations for Predictive Modeling

Equations for the combined advection-dispersion process are used to estimate the time during which a nonreactive contaminant will travel a specific distance, the pathway it will travel, and its concentration at any point. The accuracy of most predictions is only fair for typical applications, because of the complexity of the problems and the scarcity of site-specific hydrogeologic data. The lack of such data can be improved on with much less effort than is commonly presumed, especially when the cost of another round of chemical sampling is compared with the costs of additional borings, core retrievals, geophysical logging, or permeability testing.

Equations that assume a nonreactive contaminant have limited usefulness, because most contaminants react with other chemical constituents in subsurface waters and with subsurface solids in a manner that affects the rate at which they travel. Nevertheless, nonreactive advection-dispersion equations are often used to generate 'worst-case' scenarios, on the presumption that the maximum transport velocity is obtained (equal to that of pure water). This may not be as useful as it first seems. Remedial action designs require detailed breakdowns of which contaminants will arrive at extraction wells and when, how long contaminants will continue their slow release from subsurface solids, and whether the contaminants will be transformed into other chemical species by chemical or biological forces. To address these points, special terms must be added to the advection-dispersion equations.

CHEMICAL PROCESSES

As difficult as the foregoing complications may be, predicting how chemical contaminants move through the subsurface is a relatively trivial matter when the contaminants behave as ideal, nonreactive substances. Unfortunately, such behavior is limited to a small group of chemicals. The actual situation is that most contaminants will, in a variety of ways, interact with their environment through biological or chemical processes. This section focuses on the dominant chemical processes that may ultimately affect the transport behavior of a contaminant. As with the physical processes previously discussed, some of the knowledge of chemical processes has been translated into practical use in predictive models. However, the science has, in many instances, advanced well beyond what is commonly practiced. Furthermore, there is considerable evidence that suggests that numerous undefined processes affect chemical mobility. Most of the deviation from ideal nonreactive behavior of contaminants relates to their ability to change physical form by energetic interactions with other matter. The physical-chemical interactions may be grouped into: alterations in the chemical or electronic configuration of an element or molecule, alterations in nuclear composition, the establishment of new associations with other chemical species, and interactions with solid surfaces.

Chemical/Electronic Alterations

The first of these possible changes is typified by oxidation-reduction or redox reactions. This class of reactions is especially important for inorganic compounds and metallic elements because the reactions often result in changes in solubility, complexing capacity, or sorptive behavior, which directly impact on the mobility of the chemical. Redox reactions are reasonably well understood, but there are practical obstacles to applying the known science because

it is difficult to determine the redox state of the aquifer zone of interest and to identify and quantify the redox-active reactants.

Hydrolysis, elimination, and substitution reactions that affect certain contaminants also fit into this classification. The chemistry of many organic contaminants has been well defined in surface water environments. The influence of unique aspects of the subsurface, not the least of which is long residence time, on such transformations of important organic pollutants is currently under investigation. There is also a need to investigate the feasibility of promoting in-situ abiotic transformations that may enhance the potential for biological mineralization of pollutants.

Nuclear Alterations

Another chemical process interaction, which results in internal rearrangement of the nuclear structure of an element, is well understood. Radiodecay occurs by a variety of routes, but the rate at which it occurs is always directly proportional to the number of radioactive atoms present. This fact seems to make mathematical representation in contaminant transport models quite straightforward because it allows characterization of the process with a unique, well defined decay constant for each radionuclide.

A mistake that is often made when the decay constant is used in models involves the physical form of the reactant. If the decay constant is applied to the fluid concentrations and no other chemical interactions are allowed, then incorporation of the constant into the subroutine which computes fluid concentrations will not cause errors. If the situation being modeled involves chemical interactions such as precipitation, ion-exchange, or sorption, which temporarily remove the radionuclide from solution, then it is important to use a second subroutine to account for the non-solution-phase decay of the radionuclide.

Chemical Associations

The establishment of new associations with other chemical species is not as well understood. This category includes ion-exchange, complexation, and co-solvation. The lack of understanding derives from the nonspecific nature of these interactions which are, in many instances, not characterized by the definite proportion of reactants to products (stoichiometry) typical of redox reactions. While the general principles and driving mechanisms by which these interactions occur are known, the complex subsurface matrix in which they occur provides many possible outcomes and renders predictions uncertain.

Ion-exchange and complexation reactions heavily influence the mobility of metals and other ionic species in the subsurface in a reasonably predictable fashion. Their influence on organic contaminant transport, however, is not well understood. Based on

studies of pesticides and other complex organic molecules, natural organic matter (such as humic and fulvic materials) can complex and thereby enhance the apparent solubility and mobility of synthetic organic chemicals. Research is needed to define the magnitude of such interactions, not only with naturally occurring organic molecules but also with man-made organics present in contaminated environments. Research is also needed to determine if these complexes are stable and liable to transport through the subsurface. Examination of the degree to which synthetic organic chemicals complex toxic metals is also necessary. There is no theoretical objection to such interactions, and there is ample evidence that metals are moving through the subsurface at many waste sites.

Co-solvation occurs when another solvent is in the aqueous phase at concentrations that enhance the solubility of a given contaminant. This occurs in agricultural uses, for example, where highly insoluble pesticides and herbicides are mixed with organic solvents to increase their solubility in water prior to field application. There is every reason to expect similar behavior at hazardous waste sites, where a variety of solvents are typically available. At present, prediction of the extent of the solubility increases that might occur at disposal sites in the complex mixture of water and organic solvents is essentially impossible. Researchers have started examining co-solvation as an influence on pollutant transport, by working on relatively simple mixed solvent systems. This research will be extremely useful, even if the results are limited to a qualitative appreciation for the magnitude of the effects.

At the extreme, organic solvents in the subsurface may result in a phase separate from the aqueous phase. In addition to movement of this separate phase through the subsurface, contaminant mobility that involves partitioning of organic contaminants between the organic and aqueous phases must also be considered. The contaminants will move with the organic phase and will, depending on aqueous phase concentrations, be released into the aqueous phase to a degree roughly proportional to their octanol-water partition coefficients. An entire range of effects is possible, from increasing to slowing the mobility of the chemical in the subsurface relative to its migration rate in the absence of the organic phase. The equilibrium partitioning process increases the total volume of ground water affected by contaminants, by releasing a portion of the organic phase constitutents into adjacent waters. It may also interfere with transformation processes by affecting pollutant availability for reaction, or by acting as a biocidal agent to the native microflora.

Surface Interactions

Of those interactions that involve organic chemicals in the environment, none has been as exhaustively studied as sorption. Sorption studies relate, in terms of a sorption isotherm, the amount of contaminant in solution to the amount associated with the solids.

Most often the sorption term in transport models is estimated for simplicity from the assumption that the response is linear. This approximation can produce serious mass balance errors. Typically, the contaminant mass in the solution phase is underestimated and contaminant retardation is thereby overestimated. In practical applications, this means that high contaminant levels can be detected at a monitoring well long before they were predicted. To resolve the discrepancy between predicted and actual transport, most practitioners arbitrarily adjust some other poorly-characterized model parameter, for example, dispersion. This leads to the creation of a model that does not present various natural process influences in proper perspective. The predictions from such models are likely to be qualitatively, as well as quantitatively, incorrect. More widespread consideration should be given to accurate representation of non-linear sorption, particularly in transport modeling at contaminated sites.

The time dependency of the sorption process is a related phenomenon that has also been largely ignored in practical applications of sorption theory. Most models assume that sorption is instantaneous and completely reversible. A growing body of evidence argues to the contrary, not only for large organic molecules in high-carbon soils and sediments, but also for solvent molecules in low-carbon aquifer materials. Additionally, there must be some subtle interplay between sorption kinetics and ground-water flow rates which gains significance in pump-and-treat remediation efforts, where flow rates are routinely substantially increased. Constant pumpage at moderate-to-high flow rates may not allow contaminants that are sorbed to solids sufficient times of release to increase solution concentrations to maximum (equilibrium) levels prior to their removal from the aquifer. Hence, treatment costs may rise substantially due to the prolonged pumping required to remove all of the contaminants and due to the lowered efficiency of treatment of the less contaminated pumped waters.

Evidence from Superfund sites and ongoing research activities suggests that contaminant association with a solid surface does not preclude mobility. In many instances, especially in glacial tills that contain a wide distribution of particle sizes, fine aquifer materials have accumulated in the bottom of monitoring wells. Iron-based colloids have been identified in ground water downgradient from a site contaminated with domestic wastewater. If contaminants can associate with these fine particles, their mobility through the subsurface could be markedly enhanced. To determine the

significance of particle transport to pollutant movement, studies must be performed at such contaminated sites.

Although knowledge about chemical processes that function in the subsurface has been significantly expanded in recent years, this information is only slowly finding its way into practical interpretations of pollutant transport at contaminated sites. Evidence from field sites suggests that much remains to be learned about these processes.

BIOLOGICAL PROCESSES

Many contaminants that enter the subsurface environment are biologically reactive. Under appropriate circumstances they can be completely degraded to harmless products. Under other circumstances, however, they can be transformed to new substances that are more mobile or more toxic than the original contaminant. Quantitative predictions of the fate of biologically reactive substances are at present very primitive, particularly compared to other processes that affect pollutant transport and fate. This situation resulted from the ground-water community's choice of an inappropriate conceptualization of the active processes: subsurface biotransformations were presumed to be similar to biotransformations known to occur in surface water bodies. Only very recently has detailed field work revealed the inadequacy of the traditional view.

Surface Water Model Analogy

As little as five years ago ground-water scientists considered aquifers and soils below the zone of plant roots to be essentially devoid of organisms capable of transforming contaminants. As a result, there was no reason to include terms for biotransformations in transport models. Recent studies have shown that water-table aquifers harbor appreciable numbers of metabolically active microorganisms, and that these microorganisms frequently can degrade organic contaminants. It became necessary to consider biotransformation in transport models. Unfortunately, many ground-water scientists adopted the conceptual model most frequently used to describe biotransformations in surface waters.

The presence of the contaminant was assumed to have no effect on microorganism populations that degrade it. It was also assumed that contaminant concentration does not influence transformation kinetics, and that the capacity to transform the contaminant is uniformly distributed throughout the body of water under study. These assumptions are often appropriate for surface waters: contaminant concentration is usually too low and the residence time too short to allow adaptation of the microbial community to the contaminant, and the organisms that are naturally pre-adapted to the contaminant are mixed throughout the water body by

turbulence. Consequently, utilization kinetics can conveniently be described by simple first-order decay constants. In surface waters these constants are usually obtained by monitoring contaminant disappearance in water samples.

Ground-Water Biotransformations

These circumstances rarely apply to biotransformation in ground water. Contaminant residence time is usually long, at least weeks or months, and frequently years or decades. Further, contaminant concentrations that are high enough to be of environmental concern are often high enough to elicit adaptation of the microbial community. As a result, the biotransformation rate of a contaminant in the subsurface environment is not a constant, but increases after exposure to the contaminant in an unpredictable way. Careful field work has shown that the transformation rates in aquifers of typical organic contaminants, such as alkylbenzenes, can vary as much as two orders of magnitude over a meter vertically and a few meters horizontally. This surprising variability in transformation rates is not related in any simple way to system geology or hydrology.

It is difficult to determine transformation rates in subsurface material. Most microbes in subsurface material are firmly attached to solid surfaces; usually less than 1% of the total population is truly planktonic. As a result, the microbes in a ground-water sample grossly underrepresent the total microbial population in the aquifer. Thus, contaminant disappearance kinetics in a ground-water sample do not represent the behavior of the material in the aquifer. It is therefore necessary to do microcosm studies with samples representative of the entire aquifer system - a formidable technical challenge.

A Ground-Water Model

These concerns have prompted re-examination of assumptions about biotransformation implicit or explicit in traditional modeling approaches, with the realization that no one qualitative description of biotransformation can be universally applicable. Field experience has shown that the relationships that describe the biological fate of contaminants actually change within aquifers in response to geochemical constraints on microbial physiology. Rather than describing biotransformation with a continuous function applicable at all points in the aquifer, it may be more realistic to examine key geochemical parameters and to use that information to identify the relationship for biotransformation that applies at any particular point. These key parameters could include the contaminant concentration, oxygen or other electron-acceptor concentration, redox state, pH, toxicity of the contaminant or co-occurring

materials, and temperature. One such model has been evaluated in the field.

The model described an alkylbenzene and polynuclear aromatic hydrocarbon plume in a shallow water-table aquifer. Microcosm studies showed that organisms in the aquifer had adapted to these contaminants, and would degrade them very rapidly when oxygen was available. As a result of this adaptation, the hydrocarbon biodegradation rate was not controlled by any inherent property of the organisms. Rather, the physical transport processes of diffusion and dispersion seemed to dominate by controlling oxygen availability to the plume.

Because the biotransformation rate was controlled by physical processes, the actual model was very simple. Oxygen and hydrocarbon transport were simulated as conservative solutes using the U.S. Geological Survey method-of-characteristics code. A subroutine examined oxygen and hydrocarbon concentrations at each node (point located at interesecting grid lines of the model) and generated new concentrations based on oxidative metabolism stoichiometry. When the model was used to simulate the growth of the plume over time, it illustrated an important property of many such plumes. The plume grew until the rate of admixture of oxygen balanced the rate of release of hydrocarbons from the source. Afterward, the extent of the plume was at steady-state (stopped growing).

The body of field experience that can be drawn on to properly assign laws for biotransformation is growing rapidly. Transport-limited kinetics may commonly apply to releases of petroleum hydrocarbons and other easily degradable materials such as ethanol or acetone in oxygenated ground water. On the other hand, materials that can support a fermentation may follow first-order kinetics. Unfortunately, many important biotransformations in ground water are still mysteries.

Rapid field methods to determine if adaptation has occurred at a site are needed. Tools to predict whether adaptation can be expected, and to estimate the time required for adaptation if it does occur, are also needed. For systems that are limited by transport processes, field methods to estimate the aquifer processes that control mixing, such as transverse dispersion and exchange processes across the water table, are required. For systems that are limited by the intrinsic biotransformation rate, new laboratory test methods (possibly, improved microcosms) that will provide reliable estimates of the kinetic parameters are required.

In addition to being sufficiently accurate and precise, these new methods should provide estimates that are truly representative of the hydrologic unit being simulated. Because contaminants typically have long residence times in aquifers, slow transformation rates can have environmental significance. The test methods should

therefore be sufficiently sensitive to measure transformation rates that are significant in the hydrologic context being simulated. Finally, there is a need for models that go beyond simple prediction of contaminant concentrations at points in the aquifer, and forecast the concentrations produced by production wells.

ANALYTICAL AND NUMERICAL MODELS

One of the more subtly involved decisions that must be made is whether to use an analytical or a numerical model to solve a particular problem. Analytical models provide exact solutions, but many simplifying assumptions must be made for the solutions to be tractable. This places a burden on the user to test and justify the underlying assumptions and simplifications (Javendel et al, 1984). For example, the Theis equation is an analytical expression which is used to predict the piezometric head changes for pumping or injection wells in confined aquifers (Freeze and Cherry, 1979; Todd, 1980):

$$s = [Q/(4*\pi*T)] * [-0.5772 - \ln(u) + u - (u^2/(2*2!)) + (u^3/(3*3!)) - (u^4/(4*4!)) ..]$$

where:
- 's' is the change in piezometric head,
- 'Q' is the flowrate of the well,
- 'T' is the transmissivity of the aquifer, and
- 'u' = $(r^2 * s) / (4 * T * t)$;
- 'r' is the radial distance from the well,
- 'S' is the storage coefficient of the aquifer, and
- 't' is the length of time the well has been operating.

Here the principal assumptions are (Lohman, 1972):

(1) the aquifer is homogenous and isotropic,
(2) the aquifer is of infinite areal extent, relative to the effects of the well (no nearby boundaries),
(3) the well is screened over the entire saturated thickness of the aquifer,
(4) the saturated thickness of the aquifer does not vary as a result of the operation of the well,
(5) the well has an infintesimal diameter so that waters in storage in the casing represent an insignificant volume, and
(6) water is removed from or injected into the aquifer with an instantaneous change in the piezometric head.

Evaluation of the foregoing equation, which incorporates an infinite Taylor series representing the well function integral, can be accomplished graphically using type curves (Walton, 1962; Lohman, 1972). Alternatively, a simplification can be made so that the Theis equation is directly solvable (Cooper and Jacob, 1946). This is done by dropping all terms in the Taylor series with powers greater than one, and is strictly valid for cases where 'u' has a value less than 0.01 (e.g., Figure 2-2). Physically, this corresponds to a limitation on the

predictive power of the modified Theis equation; head changes predicted at locations far from the well are inaccurate, except for long durations of pumpage (i.e., approaching equilibrium or steady-state conditions).

Numerical models are much less burdened by these assumptions and are therefore inherently capable of addressing more complicated problems, but they require significantly more data and their solutions are inexact (numerical approximations). For example, the assumptions of homogeneity and isotropicity are unnecessary due to the ability to assign point (nodal) values of transmissivity and storage. Likewise, the capacity to incorporate complex boundary conditions obviates the need for the 'infinite area extent' assumption. There are, however, difficult choices facing the user of numerical models; i.e. time steps, spatial grid designs, and ways to avoid truncation errors and numerical oscillations must be chosen (Remson and others, 1971; Javendel and others, 1984). These choices, if improperly made, may result in errors unlikely to be made with analytical approaches (e.g.; mass imbalances, incorrect velocity distributions, and grid-orientation effects).

QUALITY CONTROL

These latter points signify a greater need for quality control measures when contemplating the use of numerical models. Three levels of quality control have been suggested previously (Huyakorn and others, 1984):

(1) validation of the model's mathematics by comparison of its output with known analytical solutions to specific problems,

(2) verification of the general framework of the model by successful simulation of observed field data, and

(3) benchmarking of the model's efficiency in solving problems by comparison with other models.

These levels of quality control address the soundness and utility of the model alone, and do not treat questions of its application to a specific problem. Hence, at least two additional levels of quality control appear justified:

(4) critical review of the problem conceptualization to ensure that the modeling effort considers all physical, chemical, and biological processes which may affect the problem, and

(5) evaluation of the specifics of the application; e.g., appropriateness of the boundary conditions, grid design, time steps, etc.

Validation of the mathematical framework of a numerical model is deceptively simple. The usual approach for ground-water flow models involves a comparison of drawdowns predicted by the Theis

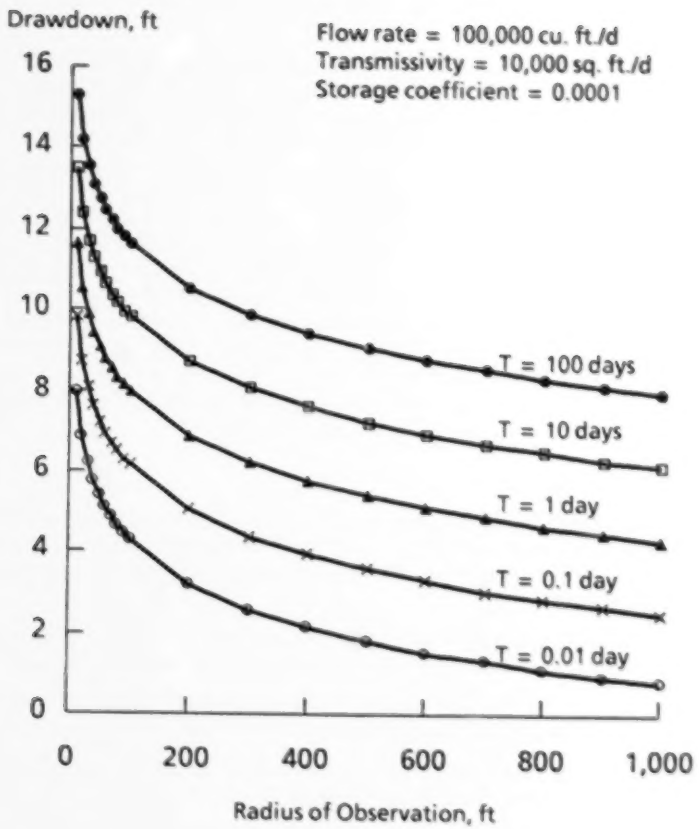

Figure 2-2. Example of plots prepared with the Jacob's approximation of the Theis analytical solution to well hydraulics in an artesian aquifer.

analytic solution to those obtained by using the model, such as depicted in Figure 2-3. The 'deceptive' part is the foreknowledge that the Theis solution can treat only a very simplified situation as compared with the scope of situations addressable by the numerical model. In other words, analytical solutions cannot test most of the capabilities of the numerical model in a meaningful way; this is particularly true with regard to simulation of complex aquifer boundaries and irregular chemical distributions.

Field verification of a numerical model consists of first calibrating the model using one set of historical records (e.g., pumping rates and water levels from a certain year), and then attempting to predict the next set of historical records. In the calibration phase, the aquifer coefficients and other model parameters are adjusted to achieve the best match between model outputs and known data; in the predictive phase, no adjustments are made (excepting actual changes in pumping rates, etc.). Presuming that the aquifer coefficients and other parameters are known with sufficient accuracy, a mismatch means that either the model is not correctly formulated or that it does not treat all of the important phenomena affecting the situation being simulated (e.g., does not allow for leakage between two aquifers when this is actually occurring).

Field verification exercises usually lead to additional data gathering efforts, because existing data for the calibration procedure are often insufficient to provide unique estimates of key parameters. This means that a 'black box' solution may be obtained, which may be good only for the records used in the calibration. For this reason, the blind prediction phase is an essential check on the uniqueness of the parameter values used. In this regard, field verification of models using datasets from controlled research experiments may be much more achievable practically.

Benchmarking routines to compare the efficiency of different models in solving the same problem have only recently become available (Ross and others, 1982; Huyakorn and others, 1984). Much more needs to be done in this area, because some unfair perceptions continue to persist regarding the ostensibly greater utility of certain modeling techniques. For example, it has been said many times that finite element models (FEM's) have an inherent advantage over finite difference models (FDM's) in terms of the ability to incorporate irregular boundaries (Mercer and Faust, 1981); the number of points (nodes) which must be used by FEM's is considerably less due to the flexible nodal spacings that are allowed. Benchmarking routines, however, show that the much longer computer time required to evaluate FEM nodes causes there to be little, if any, cost advantage for simulations of comparable accuracy.

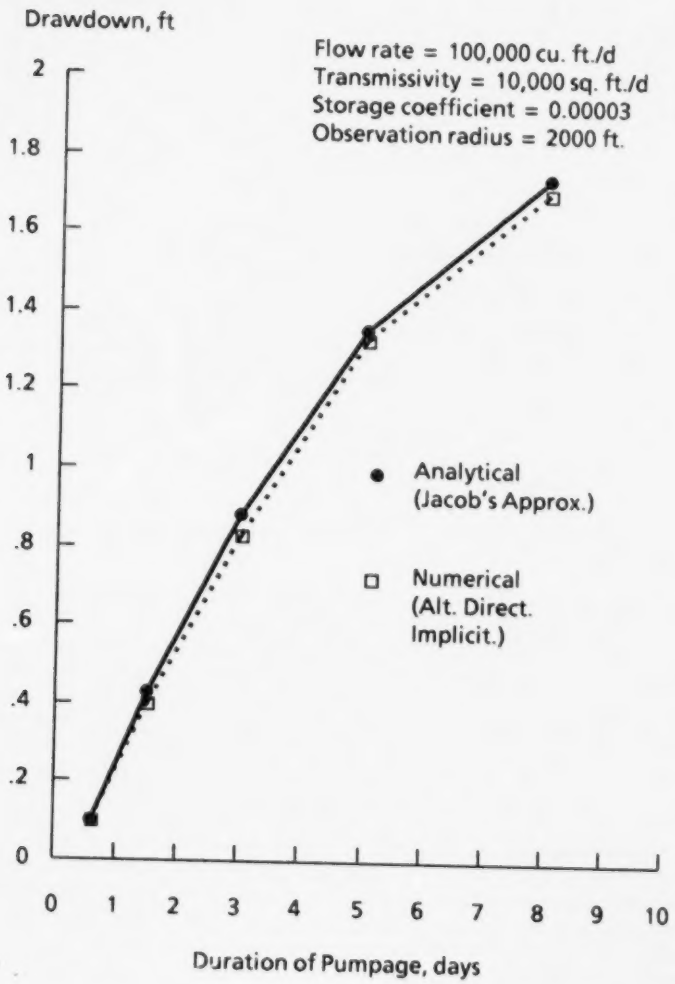

Figure 2-3. Mathematical validation of a numerical method of estimating drawdown, by comparison with an analytical solution.

CHAPTER SUMMARY

Mathematical models of subsurface contaminant transport are simplified representations of reality that incorporate a number of theoretical assumptions about the natural processes governing the transport and fate of contaminants. In order for solutions to be made tractable, further simplifications are made in applications of theory to practical problems. Hence, mathematical models produce represention that are not faithful to the true complexities of real world situations. This limitation can be partially compensated for, however, by detailed mathematical testing to determine the magnitude of errors generated by the assumptions and simplifications involved.

The application of mathematical models is also subject to considerable error in practical situations due to the lack of appropriate field determinations of natural process parameters. This source of error is not adequately addressed by sensitivity analyses or stochastic techniques for estimating uncertainty, contrary to popular beliefs. Rather, the high degree of hydrogeologic, chemical, and microbiological complexity typically present in field situations demands characterization of the magnitude of influences from various natural processes by actual field determinations.

Both the mathematics describing models and the parameter input to models must be subjected to rigorous quality control procedures. Otherwise, results from field applications of models are likely to be qualitatively, as well as quantitatively, incorrect. Quality control methodologies must recognize that accuracy and precision determinations are insufficient measures of quality. The correctness of the problem conceptualization, and the representativeness of parameter values are essential quality considerations.

CHAPTER 3
APPLICATIONS IN PRACTICAL SETTINGS

STEREOTYPICAL APPLICATIONS

As stated in preceeding sections, models are simplifications of reality that may or may not faithfully simulate the actual situation. Typically, attempts are made to mimic the effects of hydrogeologic, chemical, and biological processes in practical applications of models. These almost always involve idealizations of known or suspected features of the problem on hand. For example, the stratification of alluvial, fluvial, and glacial deposits may be assumed to occur in uniformly thick layers, despite the great variability of stratum thicknesses found in actual settings. Large blocks of each stratum are assumed to be homogeneous. Sources of chemical input are commonly assumed to have released contaminants at constant rates over the seasons and years of operational changes that the sources were active. The areal distribution of rainfall and the actual schedules of pumpage from production wells are also artificially homogenized in most modeling exercises.

All these idealizations are made necessary by a lack of the appropriate historical records and field-derived parameter estimates, and all reduce the reliability of predictions made with models. The degree of usefulness of a model is therefore directly dependent on the subjective judgements that must be made in data collection and preparation efforts prior to attempting mathematical simulations. This is true not only in a quantitative sense, but also in a qualitative sense because it is the data gathering phase of a project that begets the conceptualization on which the model will be based.

REAL-WORLD APPLICATIONS

To illustrate this point, the highlights of two very different contamination problems will be described. The first involves a relatively limited contamination incident arising from a very small source and having few contaminants. The second involves a major contamination incident arising from the operation of a chemical reprocessing facility that handled dozens of different contaminants in large amounts. The common theme that is shared by the two cases, as should also apply to virtually all cases, is one of seeking to define the relative influences of natural processes affecting contaminant transport in order to optimize the assessment

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and remediation of the problem. It is the validity of the conceptual model of what is happening at these sites that is most important, not the application of a particular mathematical model.

Field Example No. 1

The Lakewood Water District in Lakewood, Washington operates a number of wells for drinking water supply purposes. Some of the wells operated by the District, such as the two primary wells at its Ponders' Corner site (Figure 3-1), have been contaminated with low levels of volatile organic chemicals (VOC's). During the course of the investigations at the Ponder's Corner site, a number of cost-saving sampling alternatives were chosen. These related principally to the field use of a portable gas chromatograph (Organic Vapor Analyzer) for the screening of water samples and soil extracts taken while drilling monitoring wells, and to the use of selective analyses (VOCs only) of ground-water samples when initial results showed only a narrow group of contaminants to be present. The lowered analytical costs, in part, allowed for increased expenditures for geotechnical characterization of the site (Wolf and Boateng, 1983).

The geotechnical efforts, particularly the pump tests that were conducted, led to a realization that the source of the contaminants was to be found regionally downgradient (Keely and Wolf, 1983). The pumping strength of the water-supply wells, when operating, was sufficient to pull contaminants over 400 feet back upgradient of the wells they affect. This behavior was somewhat unexpected. A unique feature of the field investigation was the taking of the ground-water samples from the pumping wells concurrent with drawdown measurements obtained during pump tests (Keely, 1982).

The pump tests yielded estimates of local transmissivity and storage coefficients. They also confirmed the presence of a major aquifer boundary nearby; a buried glacial till drumlin just west of the site parallels the general direction (northwest) of regional flow. The pump tests clearly showed some anisotropy of the sediments as well; drawdown contours produced an elliptical cone of drawdown, the major axis of which was aligned with the regional flow to the north. This information resulted in modifications to the original plans, which called for drilling and constructing several monitoring wells west of the site. Instead, more monitoring wells were drilled along the north-south axis. Chemical analysis of the samples taken concurrent with drawdown measurements formed a time-series of contaminant concentrations that provided a clue to where the contaminant source was located (Keely, 1982). The time-series showed that the well nearest the downgradient edge of the wellfield was exposed to increasing contaminant levels as pumping continued, whereas the upgradient pumping well remained largely unaffected (Keely and Wolf, 1983).

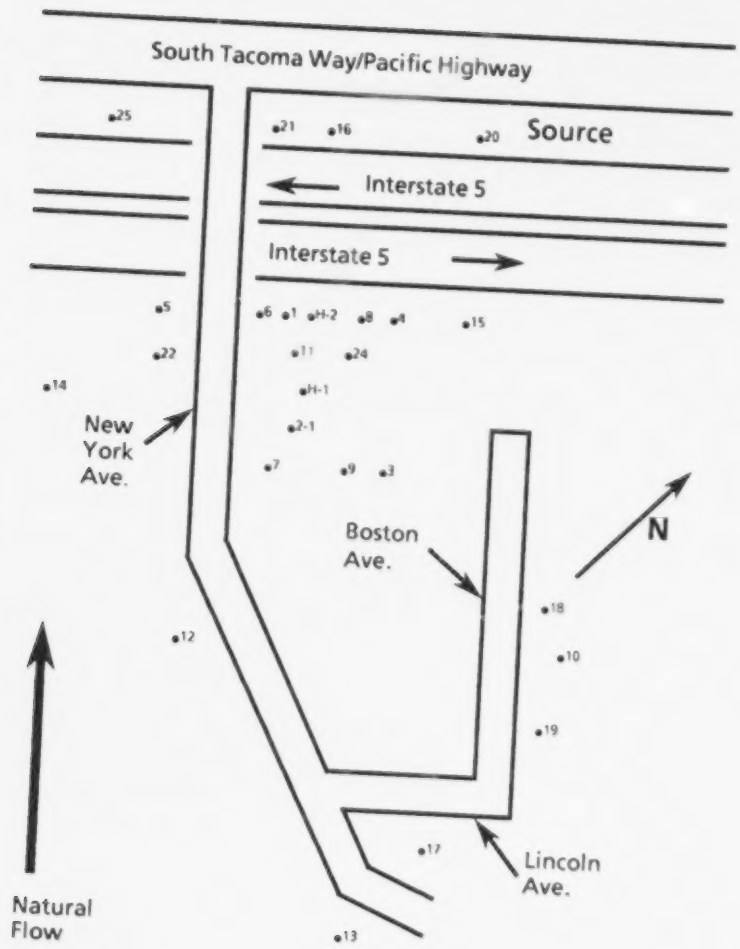


Figure 3-1. Location map for Lakewood Water District wells contaminated with volatile organic chemicals.

The hydrogeologic parameter estimates obtained from the pump tests strengthened the conceptualization of contaminants being drawn back against the regional flow because the capture zones of the pumping wells were sufficiently distorted by the local anisotropy to more than encompass the contaminant source. Without considering the anisotropic bias along the regional flow path, the estimated boundaries of the capture zone for either of the two wells marginally reached the distance to the contaminant source. The mechanism by which the two wells became contaminated seemed to be understood from a hydraulic point of view (Figure 3-2), but the chemical information did not seem to provide a consistent picture.

The source of contamination, a septic tank at a dry-cleaning facility, was found to have received large amounts of tetrachloroethylene and trichloroethylene, but no known amounts of cis- or trans-dichloroethylene; whereas the contaminated wells had relatively high concentrations of dichloroethylene. Initially it was thought that other sources might also be present and would explain the high concentrations of dichloroethylene. However, it soon became clear that recent research results regarding the potential for biotransformation of tetrachloroethylene and trichloroethylene (Wilson and McNabb, 1981) would more satisfactorily explain the observations.

Simulations of this kind of problem could be adequately performed only by contaminant transport models capable of incorporating the effects of the pumping wells on the regional flow field. More sophisticated approximations would also require the ability to account for the anisotropic and heterogeneous character of the site, the retardation of the VOC's by sorption, and their possible biotransformations. Given the highly localized nature of the contaminant source and limited extent of the plume, however, there was insufficient justification for pursuing such efforts. The resolution of the problem was possible by relatively simple source removal techniques (excavation of the septic tank and elimination of discharges).

Field Example No. 2

Similar experience with special use of geotechnical methods and state-of-the-art research findings occurred at the 20-acre Chem-Dyne solvent reprocessing site in Hamilton, Ohio (Figure 3-3). During operation of the site (1974-1980), poor waste handling practices such as onsite spillage of a wide variety of industrial chemicals and solvents, direct dischage of liquid wastes to a stormwater drain beneath the site, and mixing of incompatible wastes were engaged in routinely. These caused extensive soil and ground-water contamination, massive fish kills in the Great Miami River, and major onsite fires and explosions, respectively. The stockpiling of liquid and solid wastes resulted in thousands of badly

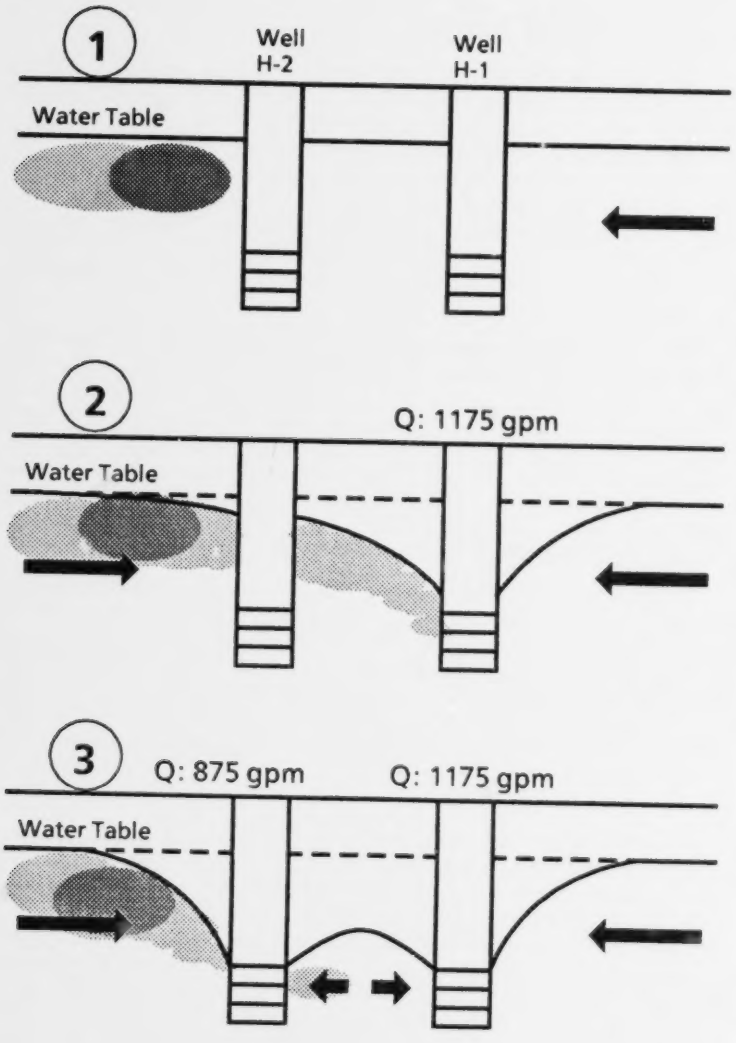


Figure 3-2. Schematic illustrating the mechanism by which a downgradient source may contaminate a production well, and by which a second well may isolate the source through hydraulic interference.

lcorroded eaking drums that posed a long-term threat to the environment (CH_2M-Hill, 1984).

The seriousness of the ground-water contamination problem became evident during the initial site survey (1980-1981), which included the construction and sampling of over twenty shallow monitoring wells (Ecology and Environment, 1982). The initial survey indicated that the contaminant problem was much more limited than was later shown to be the case (Roy F. Weston Inc., 1983, CH_2M-Hill, 1984). A good portion of the improvement in delineating the plume was brought about by an improved understanding of the natural processes controlling transport of contaminants at the site.

The initial site survey indicated that ground-water flow was generally to the west of the site, toward the Great Miami River, but that a shallow trough paralleled the river itself as a result of weak and temporary stream influences. The study concluded that contaminants would be discharged from the aquifer into the river (Ecology and Environment, 1982). That study also concluded that the source was limited to highly contaminated surface soils, and that removal of the uppermost three feet of the soil would essentially eliminate the source.

That conclusion was, however, based on faulty soil sampling procedures. The soil samples that were taken were not preserved in air-tight containers, so that most of the VOC's leaked out prior to analysis. That the uppermost soil sample showed high VOC levels is probably explained by the co-occurrence of viscous oils and other organic chemicals that may have served to entrap the VOC's. The more viscous and highly retarded chemicals did not migrate far enough into the vertical profile to exert a similar influence on samples collected at depths greater than a few feet.

Subsequent studies of the site corrected these misinterpretations by producing data from proper soil samplings and by incorporating a much more detailed characterization of the fluvial sediments and the natural flow system. In those studies vertical profile characterizations were obtained from each new borehole drilled by continuous split-spoon samples of subsurface solids; and clusters of vertically-separated monitoring wells were constructed. The split-spoon samples helped to confirm the general locations of interfingered clay lenses and clearly showed the high degree of heterogeneity of the sediments (Figures 3-4 and 3-5). While an extensive network of shallow wells confirmed earlier indications of general ground-water flow toward the river (Figure 3-6), the clusters of vertically separated wells revealed that dramatic downward gradients existed adjacent to the Great Miami River (Figure 3-7). This finding indicated that the migrating plume would not be discharged to the river, but would instead flow under the river.

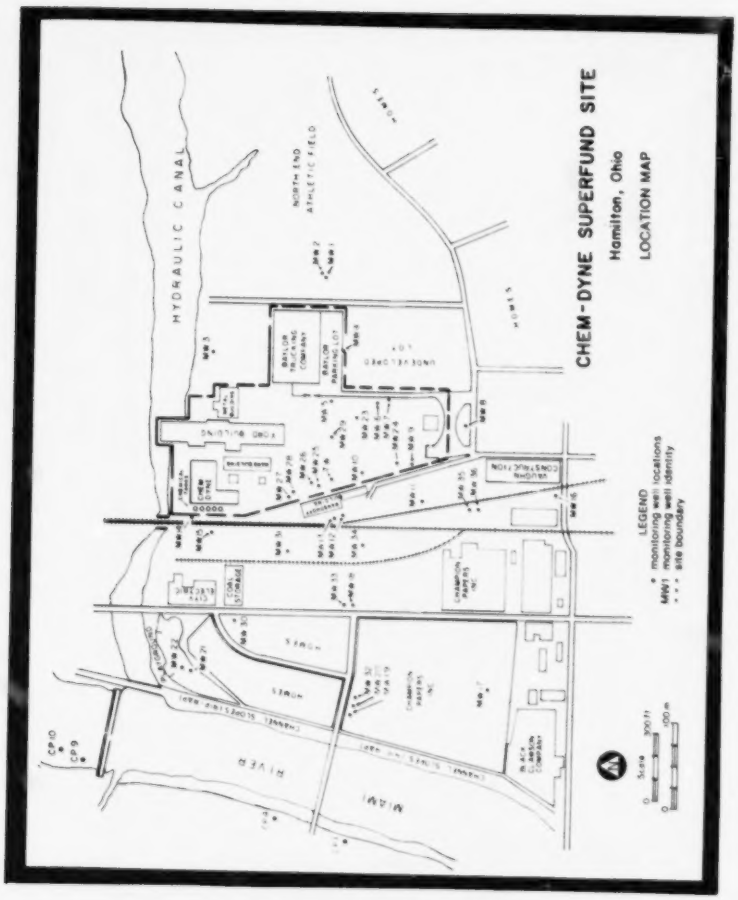


Figure 3-3. Location map for Chem-Dyne Superfund Site.

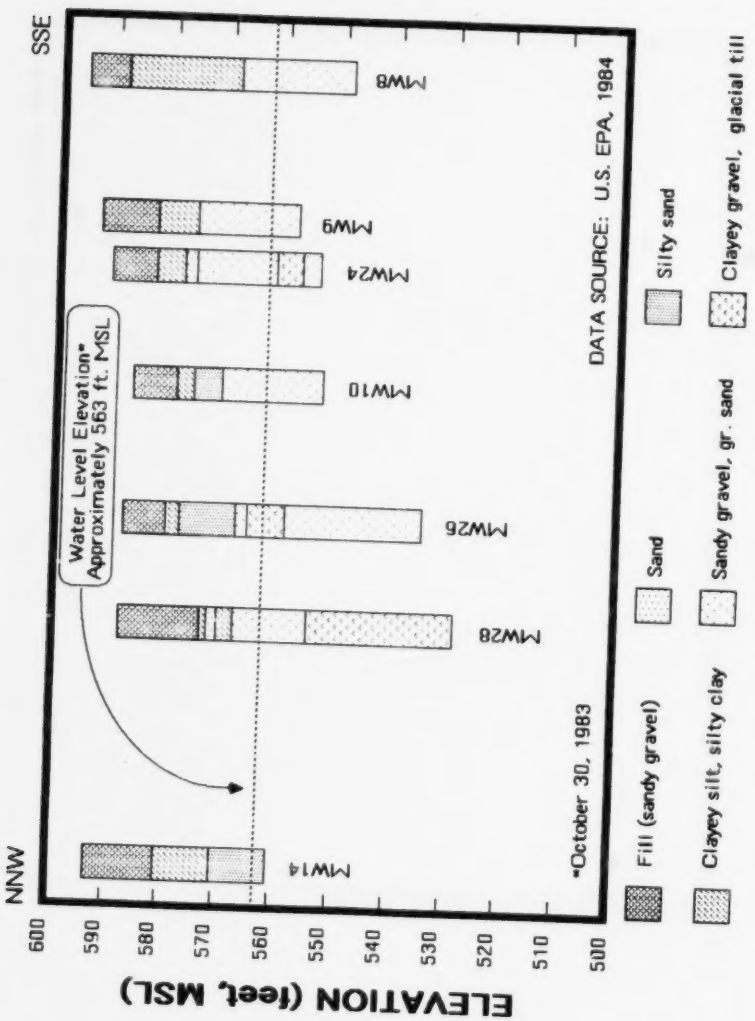


Figure 3-4. Chem-Dyne geologic cross-section along NNW-SSE axis.

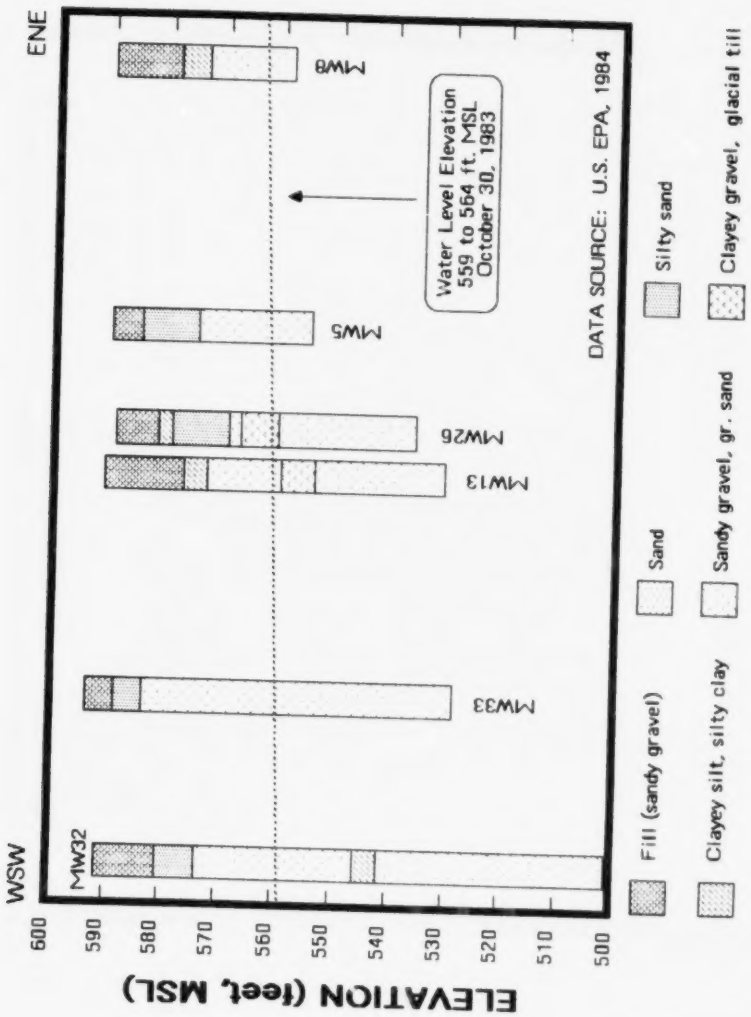


Figure 3-5. Chem-Dyne geologic cross-section along WSW-ENE axis.

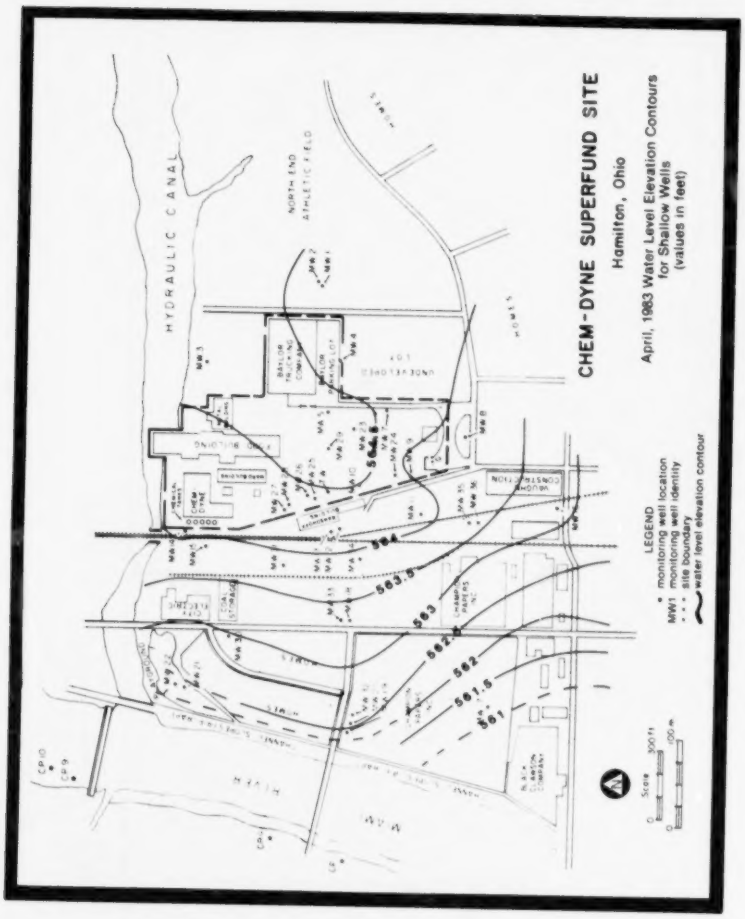


Figure 3-6. Shallow well ground-water contour map for Chem-Dyne. Flow is generally to the river (west) and down the valley (southwest).

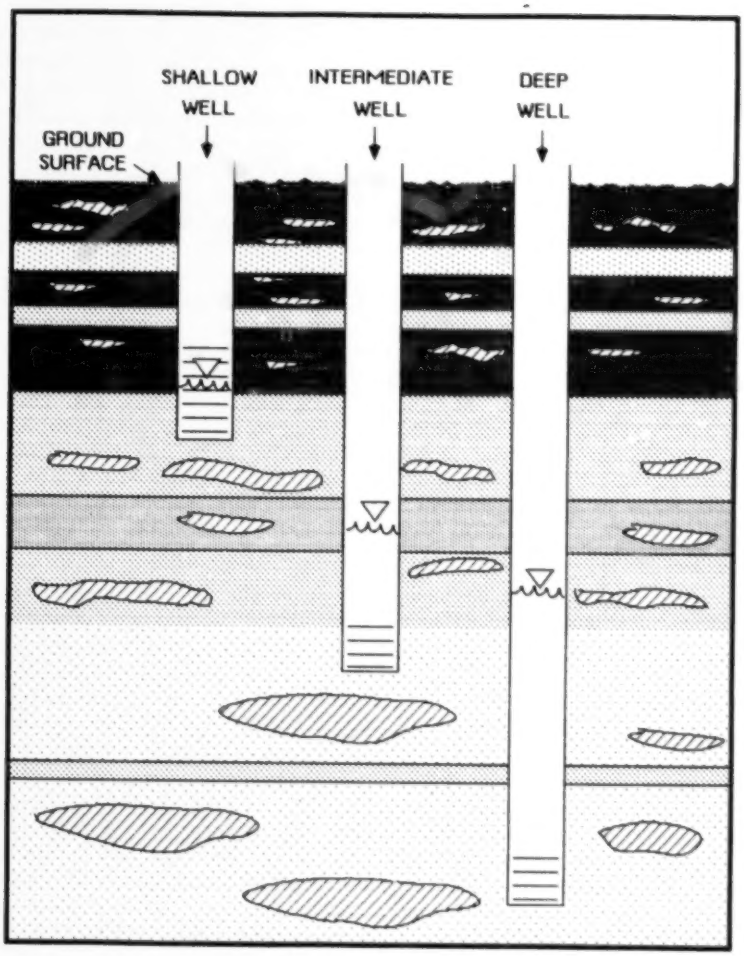


Figure 3-7. Typical arrangement of clustered, vertically-separated wells installed adjacent to Chem-Dyne and the Great Miami River.

The presence of major industrial wells on the other side of the river supported this conclusion. The plume would be drawn to greater depths in the aquifer by the locally severe downward gradient, but whether the industrial wells would actually capture the plume could not be determined. That determination would require careful evaluation of the hydrogeologic features beneath the river; something that has not been attempted because of the onset of remedial actions designed to stop the plume from reaching the river.

The field characterization efforts did, however, include the performance of a major pump test so that the hydrogeologic characteristics of the contaminated portion of the aquifer could be estimated. The pump test was difficult to arrange, because the pumping well had to be drilled onsite for reasons of potential liability and lack of property access elsewhere. The drillers were considerably slowed in their work by the need to don air-tanks when particularly contaminated subsoils were encountered because the emission of volatile fumes from the borehole presented unacceptable health risks. Since the waters which would be pumped were expected to be contaminated, it was necessary to construct ten large temporary holding tanks (100,000 gallons each) onsite to impound the waters for testing and possible treatment prior to being discharged to the local sewer system (CH_2M-Hill, 1984).

The costs and difficulty of preparing for and conducting the test were worth the effort, however. The water levels in thirty-six monitoring wells were observed during the test and yielded a very detailed picture of transmissivity variations (Figure 3-8), which has been used to help explain the unusual configuration of the plume (Figure 3-9) and which were used to guide the design of a pump-and-treat system. Storage coefficients were also estimated; and though the short duration of the test (14 hours) did not allow for definitive estimates to be obtained, it was clear that qualitative confirmation of the generally non-artesian (water-table) nature of the aquifer beneath the site was confirmed. An automated data acquisition system (computer-controlled pressure transducer system) was used to monitor the water levels and provide real-time drawdown plots of 19 of the 36 wells (Table 3-1), greatly enhancing the information obtained with only minimal manpower requirements. The benefits from conducting the pump test cannot be overemphaiszed; qualitative confirmation of lithologic information and semi-quantitative estimation of crucial parameters were obtained.

Finally, the distribution patterns of contaminant species that emerged from the investigations at Chem-Dyne were made understandable by considering research results and theories regarding chemical and microbiological influences. Once again there seemed to be evidence of transformation of tetrachloroethene (Figure 3-10) to less halogenated daughter products such as trichloroethene (Figure 3-11), dichloroethene (Figure 3-12), and vinyl chloride / monochloroethene (Figure 3-13). The relative rates

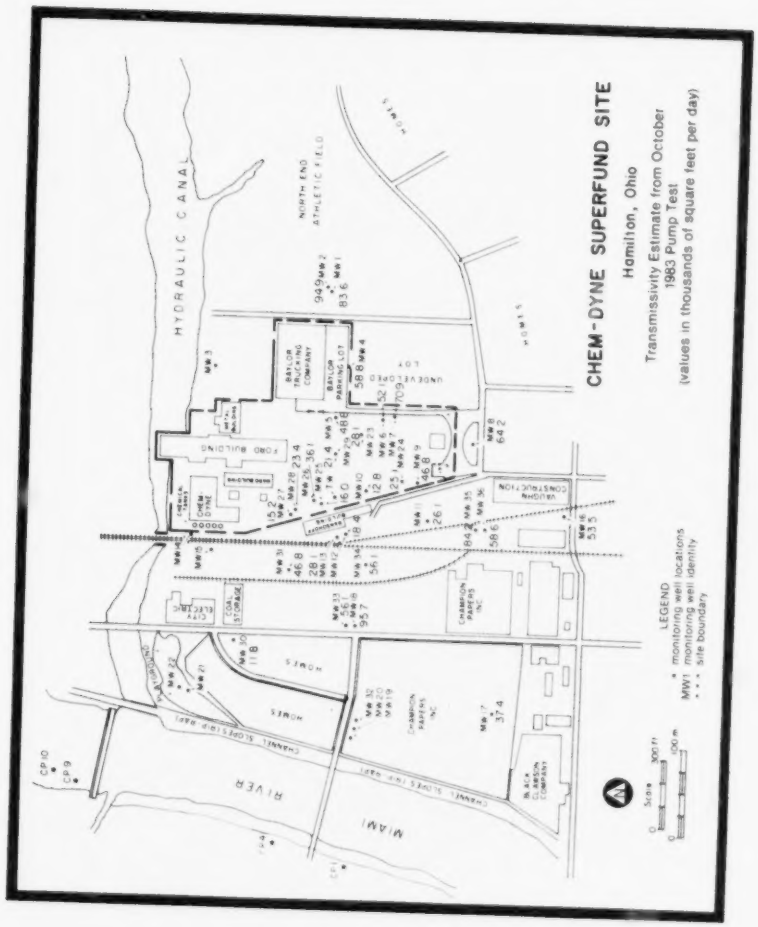


Figure 3-8. Estimates of transmissivity obtained from shallow and deep wells during Chem-Dyne test.

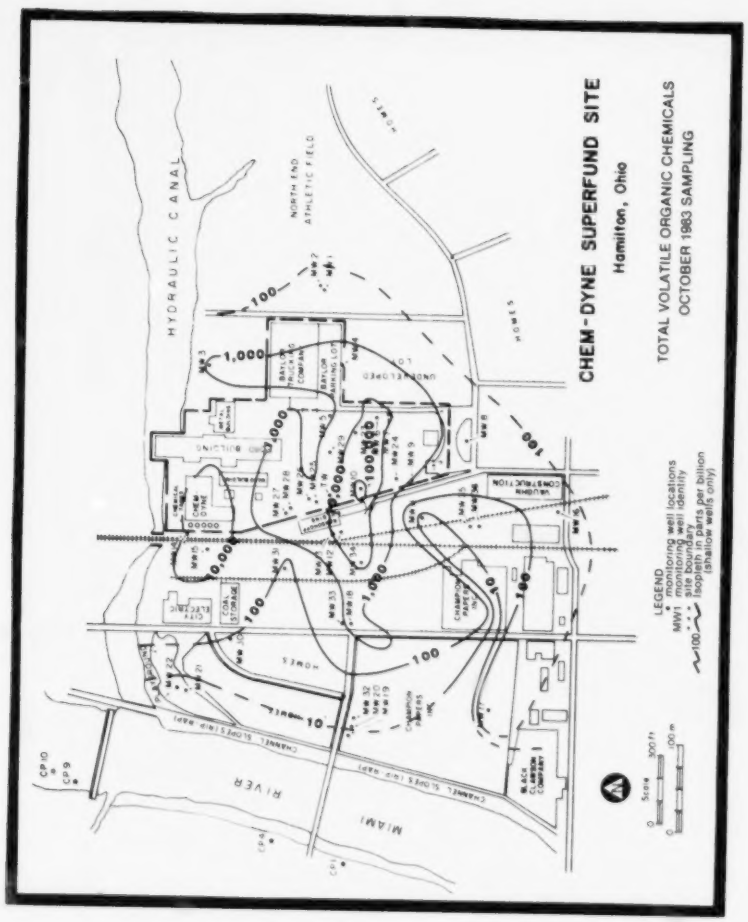


Figure 3-9. Distribution of total volatile organic chemical contamination in shallow wells at Chem-Dyne during October, 1983 sampling.

Table 3-1. Chem-Dyne Pump Test Observation Network.

Obs. Well No.	Radial Dist. (feet)	Init. Wtr. Level (ft, MSL)	Method of Measurement (type, field unit)
MW1	957	563.68	manual, electric probe
MW2	965	563.74	manual, electric probe
MW3	848	563.96	automatic, float-type
MW4	537	563.27	manual, electric probe
MW5	313	563.31	manual, electric probe
MW6	420	564.40	manual, electric probe
MW7	480	563.30	manual, electric probe
MW8	740	563.01	manual, electric probe
MW9	487	563.08	manual, electric probe
MW10	186	563.29	auto., pressure transducer
MW11	502	562.90	auto., pressure transducer
MW12	232	562.39	auto., pressure transducer
MW13	232	563.19	auto., pressure transducer
MW14	701	-	dry - no data collected
MW15	611	563.10	auto., pressure transducer
MW16	1275	562.47	manual, electric probe
MW17	1518	560.03	manual, electric probe
MW18	692	562.67	manual, electric probe
MW19	1204	559.80	automatic, float-type
MW20	1225	562.10	auotmatic, float-type
MW21	1259	561.29	manual, electric probe
MW22	1261	559.95	auto., pressure transducer
MW23	298	563.07	auto., pressure transducer
MW24	398	563.07	auto., pressure transducer
MW25	53	563.04	auto., pressure transducer
MW26	62	562.96	auto., pressure transducer
MW27	272	563.13	auto., pressure transducer
MW28	248	562.99	auto., pressure transducer
MW29	167	563.23	auto., pressure transducer
MW30	993	561.25	manual, electric probe
MW31	465	562.78	automatic, float-type
MW32	1236	559.56	auto., pressure transducer
MW33	690	562.06	auto., pressure transducer
MW34	454	562.29	auto., pressure transducer
MW35	651	562.93	auto., pressure transducer
MW36	696	562.69	manual, electric probe
Pumping Well	0 (ref. pt.)	562.97	auto., pressure transducer

of movement of these contaminants, as well as other common solvents like benzene (Figure 3-14) and chloroform (Figure 3-15), generally conformed to predictions based on sorption principles. The remediation efforts also made use of these contaminant transport principles in estimating the capacity of the treatment system needed and the length of time necessary to remove residuals from the aquifer solids (CH_2M-Hill, 1984).

During the latter stages of negotiations with the Potentially Responsible Parties (PRP's), government contractors prepared mathematical models of the flow sytem and contaminant transport at Chem-Dyne (GeoTrans, 1984). These were used to estimate the possible direction and rate of migration of the plume in the absence of remediation, the mass of contaminants removed during the various remedial options, and the effects of sorption and dispersion on those estimates. Because of the wide range of sorption properties associated with the variety of VOC's found in significant concentrations, it was necessary to select values of retardation constants that represented the likely upper- and lower-limits of sorptive effects. It was also necessary to estimate or assume the values of other parameters known to affect transport processes, such as dispersion coefficients.

While the developers of the models would be the first to acknowledge the large uncertainties associated with those modeling efforts due to lack of information about the actual history of chemical inputs and other important data, there was agreement between the government and PRP technical experts that the modeling efforts had been very helpful in assessing the magnitude of the problem and in determining minimal requirements for remediation. Consequently, modeling efforts will continue at Chem-Dyne. Data generated during the remediation phase will be used to refine models in an ongoing process so that the effectiveness of the remedial action can be evaluated properly.

PRACTICAL CONCERNS

In many ways, there may be too much confidence among those not directly involved in ground-water quality research regarding current abilities to predict transport and fate of contaminants in the subsurface. The discussions in the preceeding sections should place in proper perspective the admittedly remarkable advances that have been made in recent years by illustrating the practical and conceptual uncertainties that remain unresolved. Continuing research efforts will eventually resolve these uncertainties, but those efforts will be considerably slower if existing results are not routinely incorporated into practical situations. Research results must be tested in real-world settings because there is no alternative mechanism for validating them. Just as importantly, there are economic arguments for incorporating research findings and state-

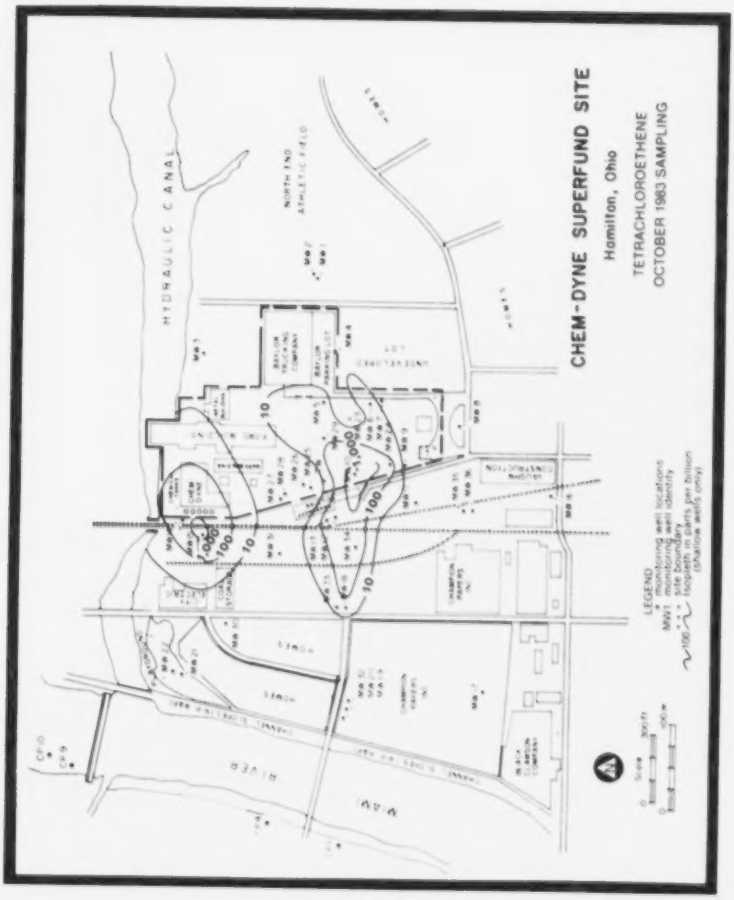


Figure 3-10. Distribution of tetrachloroethene in shallow wells at Chem-Dyne during October, 1983 sampling.

CHEM-DYNE SUPERFUND SITE
Hamilton, Ohio
TRICHLOROETHENE
OCTOBER 1983 SAMPLING
HYDRAULIC CANAL
NORTH END ATHLETIC FIELD
LOT
LOT
LOT

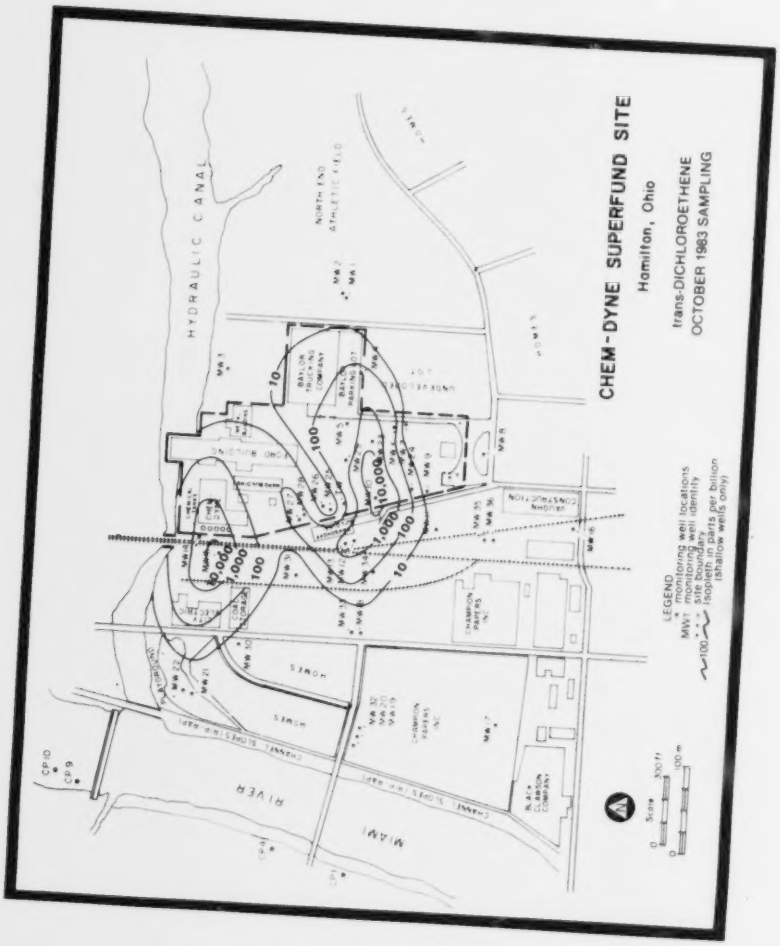


Figure 3-12. Distribution of trans-dichloroethene in shallow wells at Chem-Dyne during October, 1983 sampling.

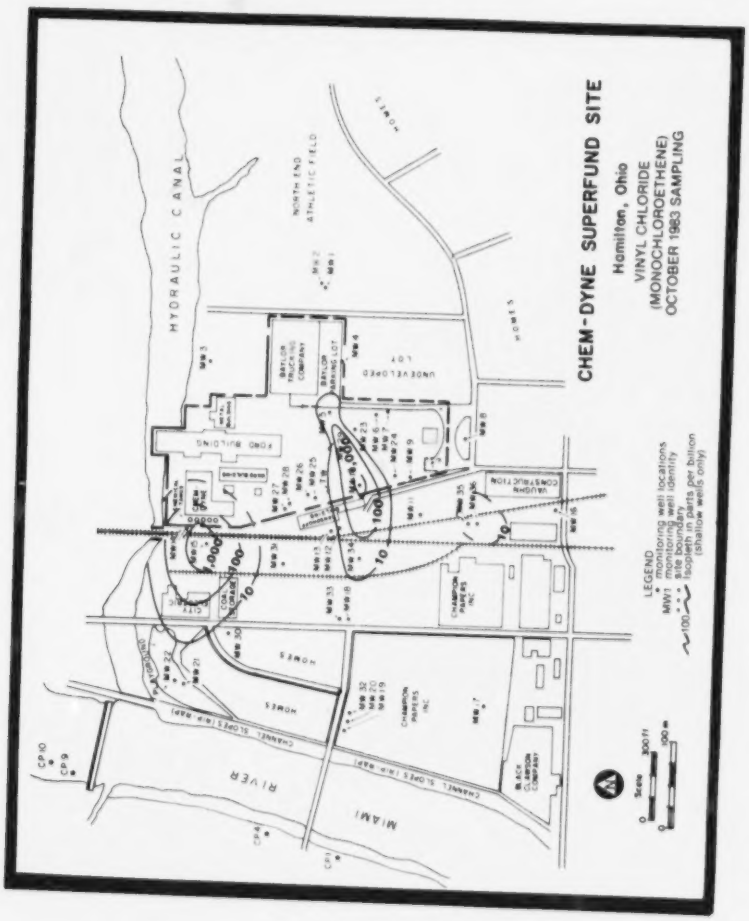


Figure 3-13. Distribution of vinyl chloride in shallow wells at Chem-Dyne during October, 1983 sampling.

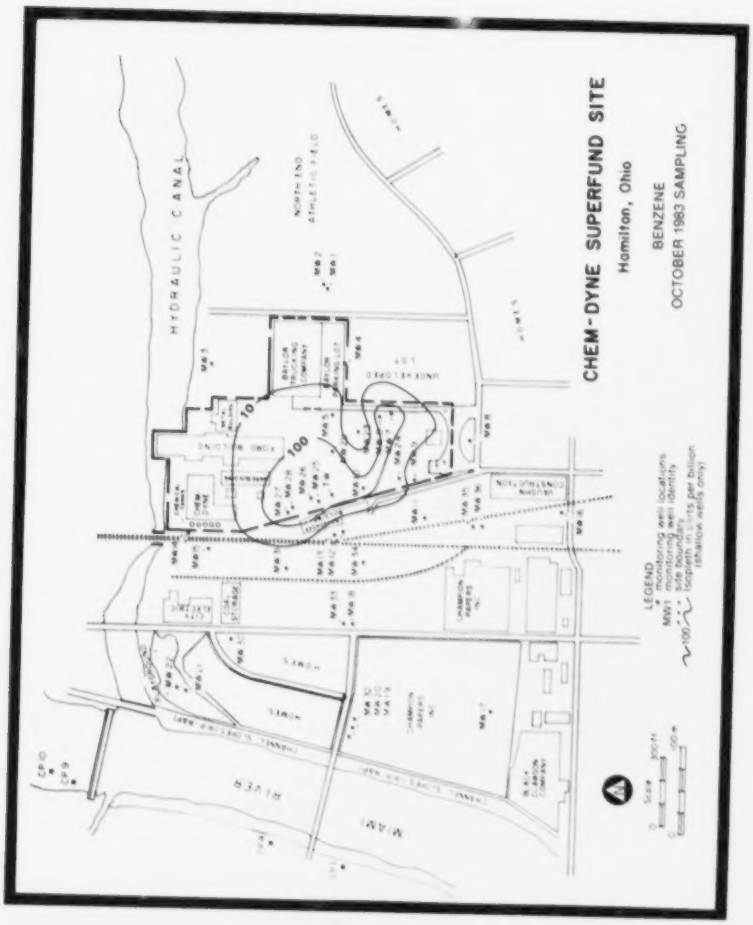


Figure 3-14. Distribution of benzene in shallow wells at Chem-Dyne during October, 1983 sampling.

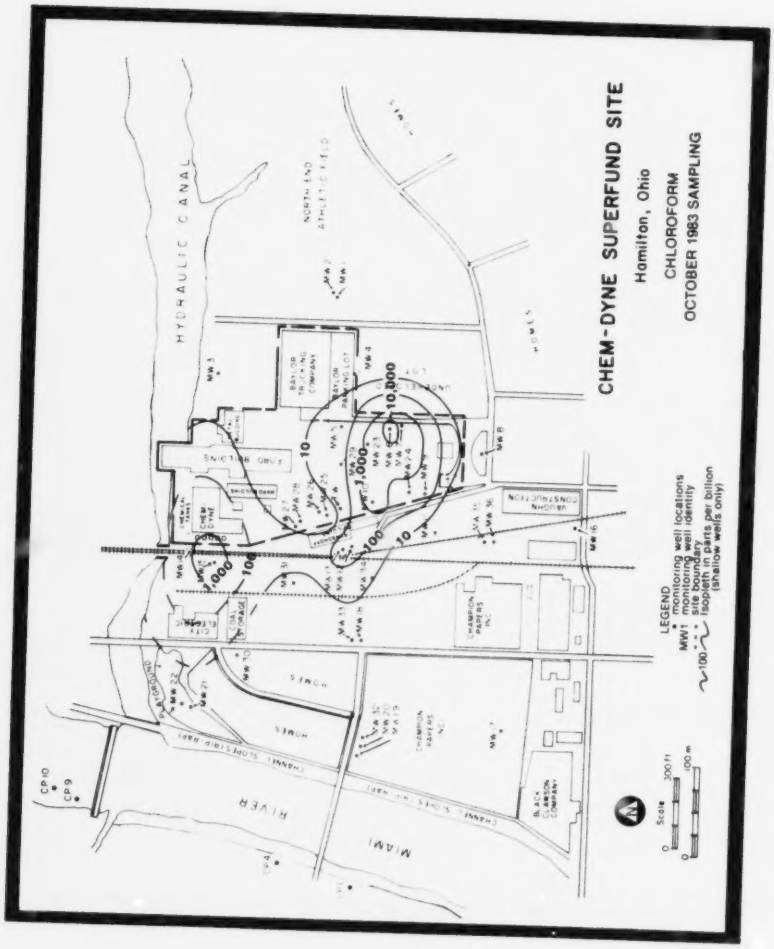


Figure 3-15. Distribution of chloroform in shallow wells at Chem-Dyne during October, 1983 sampling.

of-the-art techniques into routine contaminant investigations and remediations.

Additional effort devoted to site-specific characterizations of natural process parameters, rather than relying almost exclusively on chemical analyses of ground-water samples, can significantly improve the quality and cost effectiveness of remedial actions at such sites. To underscore this point, condensed summaries are provided of the principal activities, benefits, and shortcomings of three possible site characterization approaches: conventional (Table 3-2), state-of-the-art (Table 3-3), and state-of-the-science (Table 3-4). To further illustrate this, a qualitative assessment of desired trade-offs between characterization and clean-up costs is presented in Figure 3-16.

Table 3-2. Site Characterization Conventional Approach.

ACTIONS TYPICALLY TAKEN
Install a few dozen shallow monitoring wells
Sample and analyze numerous times for 129 + pollutants
Define geology primarily by driller's log and cuttings
Evaluate hydrology with water level maps only
BENEFITS
Rapid screening of problem
Moderate costs involved
Field and lab techniques standardized
Data analysis relatively straightforward
Tentative identification of remedial options possible
SHORTCOMINGS
True extent of problem often misunderstood
Selected remedial alternative may not be appropriate
Optimization of remedial actions not possible
Clean-up costs unpredictable and excessive
Verification of compliance uncertain and difficult

As illustrated there, some investments in specialized equipment and personnel will be necessary to make transitions to more sophisticated approaches, but those investments should be more than paid back in reduced clean-up costs. The maximum return on increased investments is expected for the state-of-the-art approach, and will diminish as the state-of-the-science approach is reached because highly specialized equipment and personnel are not widely available. It is vitally important that this philosophy be considered,

Table 3-3. Site Characterization State-of-the-Art Approach.

RECOMMENDED ACTIONS
Install depth-specific well clusters
Sample and analyze for 129 + pollutants
Analyze selected contaminants in subsequent samplings
Define geology by extensive coring/split-spoon samples
Perform limited tests on solids (grain size, clay content)
Conduct geophysical surveys (resistivity soundings, etc.)
BENEFITS
Conceptual understanding of problem more complete
Better prospect for optimization of remedial actions
Predictability of remediation effectiveness increased
Clean-up costs lowered, estimates improved
Verification of compliance soundly based, more certain
SHORTCOMINGS
Characterization costs somewhat higher
Detailed understanding of problem still difficult
Full optimization of remedial actions not likely
Field tests may create secondary problems
Demand for specialists increased

because the probable benefits in lowered total costs, health risks, and time for effective remediations can be substantial.

CHAPTER SUMMARY

It is well understood that models may be used to examine the significance of various natural processes controlling the behavior of ground water and the chemical and biological species it transports. Literally thousands of laboratory and field experiments have been conducted and interpreted with the assistance of mathematical models. Virtually all of these, however, are performed in idealized settings and are tightly controlled. There still exists the need to truly evaluate the predictive accuracy and utility of mathematical models for real-world contamination problems.

Managers are increasingly asking technical support staff to use models to interpret field data within the context of developing and optimizing alternative solutions to their problems. That this cannot be done in a meaningful way, without serious efforts to characterize natural process parameters at actual sites, must also be fully appreciated.

Table 3-4. Site Characterization State-of-the-Science Approach.

IDEALIZED APPROACH
Assume 'State-of-the-Art Approach' as starting point
Conduct tracer-tests and borehole geophysical surveys
Determine % organic carbon, exchange capacity, etc. of solids
Measure redox potential, pH, DO, etc. of fluids
Evaluate sorption-desorption behavior using select cores
Identify bacteria and assess potential for biotransformation
BENEFITS
Thorough conceptual understanding of problem obtained
Full optimization of remedial actions possible
Predictability of remediation effectiveness maximized
Clean-up costs lowered significantly, estimates reliable
Verification of compliance assured
SHORTCOMINGS
Characterization costs significantly higher
Few previous field applications of advanced theories
Field and laboratory techniques not yet standardized
Availability of specialized equipment low
Demand for specialists dramatically increased

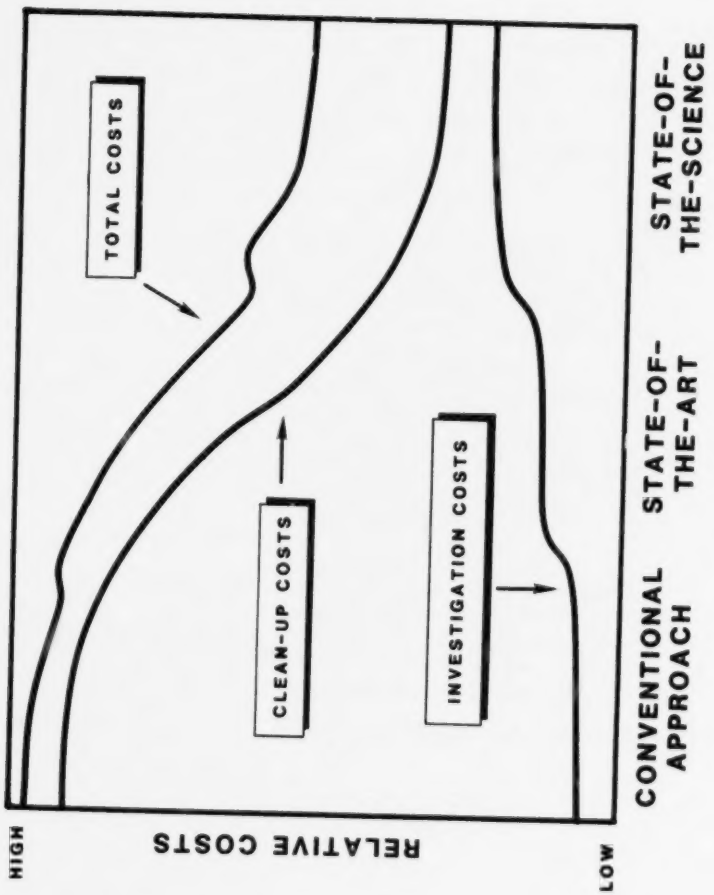


Figure 3-16. General relationship between site characterization costs and clean-up costs as a function of the characterization approach.

CHAPTER 4

LIABILITIES, COSTS, AND RECOMMENDATIONS FOR MANAGERS

INTRODUCTION

There are many texts available that describe the derivation of the theories underlying mathematical models, the technical applications of models, and related technical topics (e.g., data collection and parameter estimation techniques). Few texts treat the nontechnical issues that managers face when evaluating the possible uses of models, such as potential liabilities, costs, and communications between the modeler and management. These are, however, important considerations because many modeling efforts fail as a consequence of insufficient attention to them. This section is therefore directed to those issues.

POTENTIAL LIABILITIES

Some of the liabilities attending the use of mathematical models relate to the degree to which predictive models are relied on to set conditions for permitting or banning specific practices or products. If a model is incapable of treating specific applications properly, there may be substantially incorrect decisions made. Depending on the application, unacceptable environmental effects may begin to accumulate long before the nature of the problem is recognized. Conversely, unjustified restrictions may be imposed on the regulated community. Inappropriate or inadequate models may also cause the 're-opening clause' of a negotiated settlement agreement to be invoked when, for instance, compliance requirements that were guided by model predictions of expected plume behavior are not met.

Certain liabilities relate to the use of proprietary codes in legal settings, where the inner workings of a model may be subject to disclosure in the interests of justice. The desire for confidentiality by the model developer would likely be subordinate to the public right to full information regarding actions predicated on modelingresults. The mechanisms for protection of proprietary rights do not currently extend beyond extracted promises of confidentiality by reviewers or other interested parties. Hence, a developer of proprietary codes still assumes some risk of exposure of innovative techniques, even if the code is not pirated outright.

Yet other liabilities may arise as the result of misapplication of models or the application of models later found to be faulty. Frequently, the choices of boundary and initial conditions for a given application are hotly contested; misapplications of this kind are undoubtedly responsible for many of the reservations expressed by would-be model users. It has also happened many times in the past that a widely used and highly regarded model code was found to contain errors that affected its ability to faithfully simulate situations for which it was designed. The best way to minimize these liabilities is to adopt strict quality control procedures for each application.

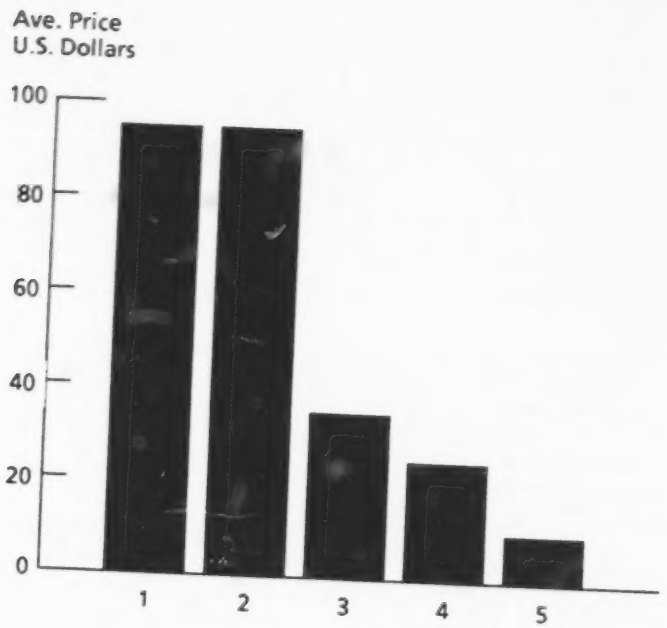
ECONOMIC CONSIDERATIONS

The nominal costs of the support staff, computing facilities, and specialized graphics' production equipment associated with numerical modeling efforts can be high. In addition, quality control activities can result in substantial costs; the determining factor in controlling these costs is the degree to which a manager must be certain of the characteristics of the model and the accuracy of its output.

As a general rule, costs are greatest for personnel, moderate for hardware, and minimal for software. The exception to this ordering relates to the combination of software and hardware purchased. An optimally outfitted business computer (e.g., VAX 11/785 or IBM 3031) costs upwards of $100,000; but it can rapidly pay for itself in terms of dramatically increased speed and computational power. A well complimented personal computer (e.g., IBM-PC/AT or DEC Rainbow) may cost $10,000; but the significantly slower speed and limited computational power may infer hidden costs in terms of the inability to perform specific tasks. For example, highly desirable statistical packages like SAS and SPSS are unavailable or available only with reduced capabilities for personal computers; many of the most sophisticated mathematical models are available in their fully capable form only on business computers.

Figure 4-1 gives a brief comparison of typical costs for software for different levels of computing power. Obviously, the software for less capable computers is cheaper, but the programs are not equivalent; so managers need to thoroughly think through what level is appropriate. If the decisions to be made are to be based on very little data, it may not make sense to insist on the most elegant software and hardware. If the intended use involves substantial amounts of data and sophisticated analyses are desired, it would be unwise to opt for the least expensive combination.

Based on experience and observation, there does seem to be an increasing drive away from both ends of the spectrum and toward the middle; that is, the use of powerful personal computers is



1 = Mainframe/business computer models
2 = Personal computer versions of mainframe models
3 = Original IBM-PC and compatibles' models
4 = Handheld microcomputer models (e.g., Sharp PC1500)
5 = Programmable calculator models (e.g., HP41-CV)

Note: Prices include software and all available documentation, reports, etc.

Source of data: International Ground Water Modeling Center

Figure 4-1. Average price per category for ground-water models from the International Ground-water Modeling Center.

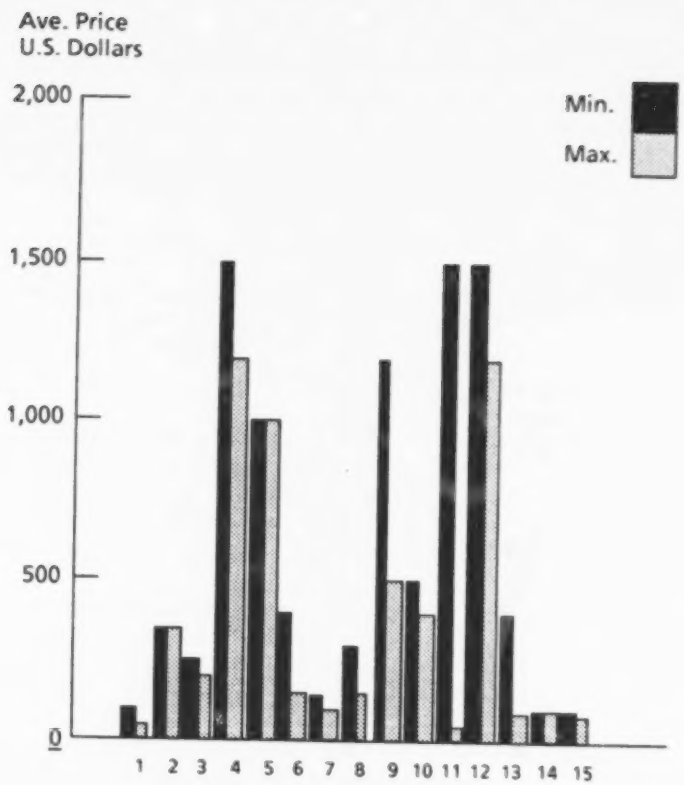
increasing rapidly, whereas the use of small programmable calculators and large business computers alike is declining.

In part, this stems from the significant improvements in the computing power and quality of printed outputs obtainable from personal computers. In part, it is due to the improved telecommunications capabilities of personal computers; they are now able to emulate the interactive terminals of large business computers so that vast computational power can be accessed and the results retrieved with no more than a phone call. Most importantly for ground-water managers, many of the mathematical models and data packages have been 'down-sized' from mainframe computers to personal computers; many more are being written directly for this market.

Since it is expected that most managers will want to explore this situation a bit more, Figure 4-2 has been prepared to provide some idea of the costs of available software and hardware for personal computers. Table 4-1 lists salary ranges and desired backgrounds for the technical support staff needed to operate such systems, based on advertisements posted in the past two years. Figure 4-3 is an attempt to place all of the nominal costs in perspective.

The technical considerations discussed in previous sections indicate that the desired accuracy of the modeling effort directly affects the total costs of mathematical simulations. Thus managers will want to determine the incremental benefits gained by increased expenditures for more involved mathematical modeling efforts. There are many economic theories which can be helpful in determining the incremental benefits gained per increased level of investment. The most straightforward of these are the cost-benefit approaches commonly used to evaluate the economic desirability of water resource projects. There are two generalized approaches in common practice: the 'benefit/cost ratio' method and the 'net benefit' method.

The benefit/cost ratio method involves tallying the economic value of all benefits and dividing that sum by the total cost involved in generating those benefits (i.e.; B/C = ?). A ratio greater than one is required for the project to be considered viable, though there may be sociopolitical reasons for proceeding with projects that do not meet this criterion. Consider the example where a project is about to get underway and has gained considerable social or political momentum when the initial cost estimates begin to prove too low. Not proceeding or substantially altering the work may be economically wise; however, such a decision may be viewed as a breach of faith by the public. Regardless of how this kind of situation evolves, it is not uncommon for certain costs to be forgiven or subsidized and this muddies the picture for incremental benefits or trade-off analyses.



1. International Ground Water Modeling Ctr.
2. Computapipe Co.
3. Data Services, Inc.
4. GeoTrans, Inc.
5. Hydrosoft, Inc.
6. In Situ, Inc.
7. Irrisco Co.
8. Koch and Assoc.
9. KRS Enterprises, Inc.
10. Michael P. Spinks Co.
11. RockWare, Inc.
12. Solutech Corp.
13. T. A. Prickett & Assoc.
14. James S. Ulrick Co.
15. Watershed Research, Inc.

Figure 4-2. Price ranges for IBM-PC ground-water models available from various sources.

Table 4-1. **Desired backgrounds and salary ranges advertised for positions requiring ground-water modeling.**

Position Title:	Hydrogeologist (Argonne Nat'l. Lab.)
Salary Offered:	$31,619 - $48,876
Desired Bkgrnd:	familiarity and experience in field testing and monitoring of ground-water flow and the use of numerical models
Position Title:	Hydrologic Modeler (Univ. of Wisonsin)
Salary Offered:	$23,000 - $25,000
Desired Bkgrnd:	primary strength in application of numerical models to ground-water flow and chemical transport; strong chemical background
Position Title:	Soil Scientist (U.S. EPA)
Salary Offered:	$31,619 - $41,105
Desired Bkgrnd:	knowledge of (i) soil physics, (ii) processes governing transport and fate of chem. and bio. species, (iii) math, statistics and geostat.; and the ability to develop computer codes
Position Title:	Ground-Wtr .Hydrol. (Inyo Co. Wtr .Dept., CA)
Salary Offered:	starting up to $32,000
Desired Bkgrnd:	at least three years experience including field work, surface/ground-water resource eval., environ. assess., flow modeling, FORTRAN
Position Title:	Hydrogeologist (S.W. Texas State Univ.)
Salary Offered:	$24,444 - $30,096
Desired Bkgrnd:	academic training in hydrogeology, min. 2 years experience, knowledge of limestone aquifers and computer operations
Position Title:	Geochemist (U.S. Nuclear Regulatory Comm.)
Salary Offered:	$23,170 - $41,105
Desired Bkgrnd:	knowledge of solute and radionuclide transport, including speciation, attenuation (sorption) numerical modeling
Position Title:	Hydrogeol./Civil.Engr. (typical consulting firm)
Salary Offered:	'conmmensurate with experience'
Desired Bkgrnd:	strong background in applied ground-water flow and contaminant transport modeling, knowledge of federal/state regulations

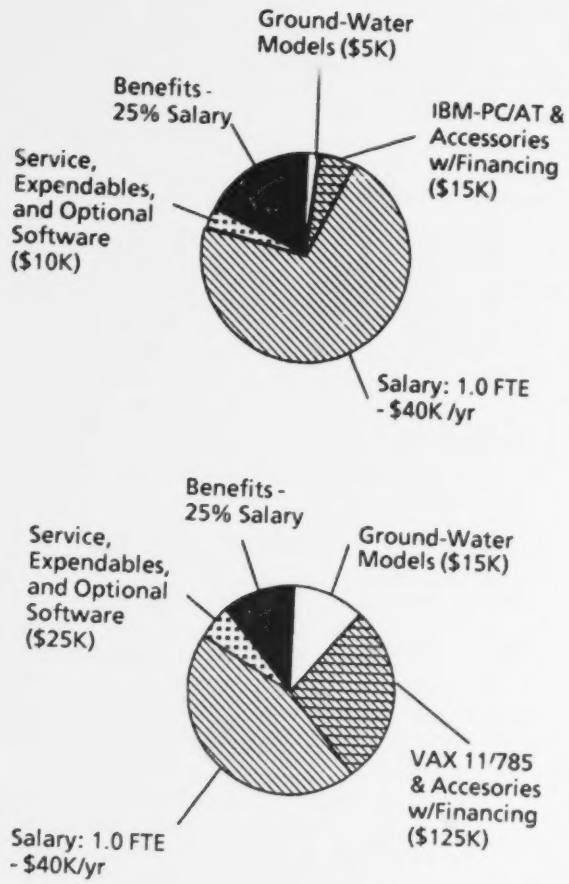


Figure 4-3. Costs of sustaining ground-water modeling capabilities at two different computing levels for a five-year period.

The 'net benefit' method involves determining the arithmetic difference of the total benefits and total costs (i.e.; B-C = ?). Here the obvious criterion is that the proposed work result in a situation where total benefits exceed total costs. This approach is most often adopted by profit-making enterprises, because they seek to maximize the difference as a source of income. The ratio method, by contrast, has long been used by government agencies and other non-profit organizations because they seek to show the simple viability of their efforts irrespective of the costs involved.

In a very real sense, then, these two general economic assessment methods stem from different philosophies. They share many common difficulties and limitations, however. For example, there is a need to predict the present worth of future costs and to amortize benefits over the life of a project. The mechanics of such calculations are well known, but they necessarily involve substantial uncertainties. For example, the present worth of a series of equal payments for equipment or software can be computed by (White and others, 1984):

$$P = A * [((1 + i)^n - 1) / (i * (1 + i)^n)]$$

where: P is the present worth,
A is the series payment each interest period,
i is the interest rate per period, and
n is the number of interest periods.

Note, however, that the interest rate must be estimated; this has fluctuated widely in the past two decades as a result of inflationary and recessionary periods in our economy. The significance of this is that a small difference in the interest rate results in tremendous differences in the present worth estimate because of the exponential nature of the equation.

It is also possible to compute the future worth of a present investment, to calculate the percentage of worth annually acquired through single payments or serial investments, and so on. One should be aware that these methods of calculating costs belong to the general family of 'single-objective', or 'mutually-exclusive alternative' analyses which presuppose that the cost of two actions is obtained by simple addition of their singly-computed costs. In other words, the efforts being evaluated are presumed to have no interactions. For some aspects of ground-water modeling efforts this assumption may not be valid; e.g., one may not be able to specify software and hardware costs independently. In addition, these methods rely on the 'expected value concept', wherein the expected value of an alternative is viewed as the single product of its effects and the probability of their occurence. This means that high-risk, low-probability alternatives and low-risk, high-probability alternatives have the same expected value.

To overcome these difficulties it is necessary to use methods which can incorporate functional dependencies between various alternatives and which do not rely on the expected value concept, such as multi-objective decision theories (Asbeck and Haimes, 1984; Haimes and Hall, 1974; Haimes, 1981). A conceivable use would be the estimation of lowered health risks associated with various remedial action alternatives at a hazardous waste site. In such a case the output of a contaminant transport model would be used to provide certain inputs (i.e., water levels, contaminant concentrations, etc.) to a health effects model, and it would convert these into the inputs for the multiobjective decision model (e.g., probability of additional cancers per level of contaminant). The primary difficulty with these approaches to cost-benefit analyses is in clearly formulating the overall probabilities of the alternatives, so that the objectives which are to be satisfied may be ranked in order of importance. A related difficulty is the need to specify the functional form of the inputs (e.g., the 'population distribution function' of pumpage rates or contaminant levels). Historical records about the inputs may be insufficient to allow their functional forms to be determined.

Another problem compounding the cost-benefit analysis of mathematical modeling efforts relates to the need to place an economic value on intangibles. For example, the increased productivity a manager might expect as a result of rapid machine calculations replacing hand calculations may not be as definable in terms of the improved quality of judgements made as it is in terms of time released for other duties. Similarly, the estimation of improved ground-water qaulity protection benefits may necessitate some valuation of the human life and suffering saved (rather nebulous quantities). Hence, there is often room for considerable 'adjustment' of the values of costs and benefits. This flexibility can be used inappropriately to improve otherwise unsatisfactory economic evaluations. Lehr (1986) offers a scathing indictment of the Tennessee Valley Authority for what he described as an 'extreme injustice', perpetrated by TVA in the form of hydroelectric projects which have 'incredibly large costs and negative cost benefit ratios'.

Finally, some costs and benefits may be incorrectly evaluated because the data on which they are based are probabilistic and this goes unrecognized. For instance, we often know the key parameters affecting ground-water computations (i.e., hydraulic conductivity) only to within an order-of-magnitude due to data collection limitations. In these situations great caution must be exercised.

On the one hand, excessive expenditures may be made to ensure that the model 'accurately' simulates observed (though inadequate) data. On the other, the artistic beauty of computer generated results sometimes generates its own sense of what is 'right', regardless of apparent clashes with common sense. The reason the basic data are uncertain is very important. Costs are not uncertain just because of

lack of information about future interest rates; many times expectations are not realized because of societal and technological changes. Miller (1980) noted that EPA overestimated the cost of compliance with its proposed standard for vinyl chloride exposure by 200 times the actual costs.

MANAGERIAL CONSIDERATIONS

The return on investments made to use mathematical models rests principally with the training and experience of the technical support staff applying the model to a problem and on the degree of communication between those persons and management. In discussing the potential uses of computer modeling for ground-water protection efforts, Faust and others (1981) summarized by noting that 'the final worth of modeling applications depends on the people who apply the models'. Managers should be aware that a fair degree of specialized training and experience are necessary to develop and apply mathematical models, and relatively few technical support staff can be expected to have such skills presently (van der Heijde and others, 1985). This is due in part to the need for familiarity with a number of scientific disciplines, so that the model may be structured to faithfully simulate real-world problems.

What levels of training and experience are necessary to apply mathematical models properly? Do we need 'Rennaissance' specialists or can interdisciplinary teams be effective? The answers to these questions are not clear-cut. From experience it is easy to see that the more informed an individual is, the more effective he or she can be. It is doubtful, however, that any individual can master each discipline with the same depth of understanding that specialists in those fields have. What is clear is that some working knowledge of many sciences is necessary so that appropriate questions may be put to specialists, and so that some sense of integration of the various disciplines can evolve. In practice this means that ground-water modelers have a great need to become involved in continuing education efforts. Managers should expect and encourage this because the benefits to be gained are tremendous, and the costs of not doing so may be equally large. An ability to communicate effectively with management is essential also.

Just as is the case with statistical analyses, an ill-posed problem yields answers to the wrong questions ('I know you heard what I said, but did you understand what I meant?'). Some of the questions managers should ask technical support staff, and vice versa, to ensure that the solution being developed is appropriate to the actual problem are listed in Tables 4-2 through 4-4. Table 4-2 consists of 'screening level' questions, Table 4-3 addresses the need for correct conceptualizations, and Table 4-4 is comprised of sociopolitical concerns.

Table 4-2. Screening-level questions to help ground-water managers focus mathematical modeling efforts.

General Problem Definition

(1) What are the key issues; quantity, quality, or both?
(2) What are the controlling geologic, hydrologic, chemical and biological features?
(3) Are there reliable data (proper field scale, quality controlled, etc.) for preliminary assessments?
(4) Do we have the model(s) needed for appropriate simulations?

Initial Responses Needed

(1) What is the time-frame for action (imminent or long-term)
(2) What actions, if taken now, can significantly delay the projected impacts?
(3) To what degree can mathematical simulations yield meaningful results for the action alternatives, given available data?
(4) What other techniques or information (generic models, past experiences, etc.) would be useful for initial estimates?

Strategies for Further Study

(1) Are the critical data gaps identified; if not, how well can simulations determine the specific data needs?
(2) What are the trade-offs between additional data and increased certainty of the simulations?
(3) How much additional manpower and resources are necessary for further modeling efforts?
(4) How long will it take to produce useful simulations, including quality control and error-estimation efforts?

On another level of communication, managers should appreciate how difficult it will be to explain the results of complicated models to non-technical audiences such as in public meetings and courts of law. Many scientists find it a trying exercise to discuss the details of their labors without the convenience of the jargon of their discipline. Some of the more useful means of overcoming this limitation involve the production of highly simplified audio-visual aids, but this necessarily involves a great deal of work. The efforts which will be required to sell purportedly self-explanatory graphs from computer simulations may rival the efforts spent on producing the simulations initially.

Table 4-3. Conceptualization questions to help ground-water managers focus mathematical modeling efforts.

Assumptions and Limitations

(1) What are the assumptions made, and do they cast doubt on the model's projections for this problem?
(2) What are the model's limitations regarding the natural processes controlling the problem; can the full spectrum of probable conditions be addressed?
(3) How far in space and time can the results of the model simulations be extrapolated?
(4) Where are the weak spots in the application, and can these be further minimized or eliminated?

Input Parameters and Boundary Conditions

(1) How reliable are the estimates of the input parameters; are they quantified within accepted statistical bounds?
(2) What are the boundary conditions, and why are they appropriate to this problem?
(3) Have the initial conditions with which the model is calibrated been checked for accuracy and internal consistency?
(4) Are the spatial grid design(s) and time-steps of the model optimizedfor this problem?

Quality Control and Error Estimation

(1) Have these models been mathematically validated against other solutions to this kind of problem?
(2) Has anyone field verified these models before, by direct applications or simulation of controlled experiments? Have these models been mathematically validated against other solutions to this kind of problem?
(3) How do these mdoels compare with others in terms of computational efficiency, and ease of use or modification?
(4) What special measures are being taken to estimate the overall errors of the simulations?

CHAPTER SUMMARY

Mathematical models can be helpful tools to managers of ground-water resource programs. Models may be used for testing hypotheses about conceptualizations and to generate better understanding of important physical, chemical, and biological processes which affect ground-water resources. The possible outcomes of complex problems can be addressed in great detail, if

Table 4-4. Sociopolitical questions to help ground-water managers focus mathematical modeling efforts.

Demographic Considerations

(1) Is there a larger population endagered by the problem than we are able to provide sufficient responses to?
(2) Is it possible to present the model's results in both non-technical and technical formats, to reach all audiences?
(3) What role can modeling play in public information efforts?
(4) How prepared are we to respond to criticism of the model(s)?

Political Constraints

(1) Are there non-technical barriers to using this model, such as 'tainted by association' with a controversy elsewhere?
(2) Do we have the cooperation of all involved parties in obtaining the necessary data and implementing the solution?
(3) Are similar technical efforts for this problem being undertaken by friend or foe?
(4) Can the results of the model simulations be turned against us; are the results ambiguous or equivocal?

Legal Concerns

(1) Will the present schedule allow all regulatory requirements to be met in a timely manner?
(2) If we are dependent on others for key inputs to the model(s), how do we recoup losses stemming from their non-performance?
(3) What liabilities are incurred for projections which later turn out to be misinterpretations originating in the model?
(4) Do any of the issues relying on the application of the model(s) require the advice of attorneys?

adequate data are available. Mathematical modeling is neither simple nor impossible. Its successful application, however, relies heavily on the expertise of the modeler and the degree of communication with management.

The use of mathematical models in the decision-making process means that the user will inevitably incur certain liabilities. Anticipation of problem areas and some sensitivity to the possible misuses of models will greatly minimize potential liabilities, as will rigorous quality control programs. A number of direct and indirect

costs attend the use of models, not the least of which involve efforts to obtain and retain specialized experts.

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